FIG. 1

		Atom Type	Res.		X	Y	Z	OCC	B	MOL
ATOM	1	C	GLY	1	69.326	51.394	17.320	1.00	31.75	CPS1
ATOM	2	O	GLY	1	69.833	51.813	16.277	1.00	31.77	CPS1
ATOM	3	N	GLY	1	70.959	52.760	18.620	1.00	35.87	CPS1
ATOM	4	CA	GLY	1	70.031	51.571	18.653	1.00	32.48	CPS1
ATOM	5	N	ILE	2	68.153	50.776	17.347	1.00	28.47	CPS1
ATOM	6	CA	ILE	2	67.404	50.567	16.121	1.00	26.25	CPS1
ATOM	7	CB	ILE	2	66.717	49.195	16.134	1.00	25.90	CPS1
ATOM	8	CG2	ILE	2	65.743	49.071	14.958	1.00	25.20	CPS1
ATOM	9	CG1	ILE	2	67.788	48.104	16.055	1.00	28.68	CPS1
ATOM	10	CD1	ILE	2	67.235	46.714	16.136	1.00	29.70	CPS1
ATOM	11	C	ILE	2	66.379	51.671	15.959	1.00	24.77	CPS1
ATOM	12	O	ILE	2	65.635	51.988	16.893	1.00	24.24	CPS1
ATOM	13	N	TYR	3	66.358	52.282	14.781	1.00	23.49	CPS1
ATOM	14	CA	TYR	3	65.407	53.355	14.515	1.00	23.75	CPS1
ATOM	15	CB	TYR	3	65.923	54.291	13.420	1.00	25.80	CPS1
ATOM	16	CG	TYR	3	64.952	55.408	13.087	1.00	28.36	CPS1
ATOM	17	CD1	TYR	3	64.870	56.552	13.887	1.00	30.78	CPS1
ATOM	18	CE1	TYR	3	63.950	57.569	13.608	1.00	33.13	CPS1
ATOM	19	CD2	TYR	3	64.090	55.307	11.999	1.00	29.71	CPS1
ATOM	20	CE2	TYR	3	63.166	56.313	11.709	1.00	32.64	CPS1
ATOM	21	CZ	TYR	3	63.102	57.444	12.517	1.00	34.23	CPS1
ATOM	22	OH	TYR	3	62.204	58.454	12.225	1.00	36.12	CPS1
ATOM	23	C	TYR	3	64.075	52.766	14.068	1.00	23.33	CPS1
ATOM	24	O	TYR	3	63.022	53.193	14.517	1.00	24.16	CPS1
ATOM	25	N	GLY	4	64.130	51.792	13.166	1.00	21.11	CPS1
ATOM	26	CA	GLY	4	62.909	51.182	12.672	1.00	20.13	CPS1
ATOM	27	C	GLY	4	63.216	49.984	11.799	1.00	19.67	CPS1
ATOM	28	O	GLY	4	64.354	49.800	11.371	1.00	18.21	CPS1
ATOM	29	N	ILE	5	62.211	49.145	11.562	1.00	18.70	CPS1
ATOM	30	CA	ILE	5	62.402	47.985	10.704	1.00	17.69	CPS1
ATOM	31	CB	ILE	5	62.470	46.666	11.510	1.00	18.45	CPS1
ATOM	32	CG2	ILE	5	63.538	46.799	12.610	1.00	17.74	CPS1
ATOM	33	CG1	ILE	5	61.103	46.329	12.127	1.00	17.47	CPS1
ATOM	34	CD1	ILE	5	61.097	44.956	12.830	1.00	18.74	CPS1
ATOM	35	C	ILE	5	61.225	47.936	9.736	1.00	17.16	CPS1
ATOM	36	O	ILE	5	60.170	48.525	10.001	1.00	16.88	CPS1
ATOM	37	N	GLY	6	61.414	47.248	8.616	1.00	16.81	CPS1
ATOM	38	CA	GLY	6	60.353	47.163	7.632	1.00	16.27	CPS1
ATOM	39	C	GLY	6	60.398	45.846	6.893	1.00	17.21	CPS1
ATOM	40	O	GLY	6	61.468	45.303	6.623	1.00	17.76	CPS1
ATOM	41	N	LEU	7	59.220	45.345	6.555	1.00	17.08	CPS1
ATOM	42	CA	LEU	7	59.085	44.080	5.858	1.00	18.22	CPS1
ATOM	43	CB	LEU	7	58.631	43.006	6.857	1.00	18.52	CPS1
ATOM	44	CG	LEU	7	58.266	41.643	6.270	1.00	18.46	CPS1
ATOM	45	CD1	LEU	7	59.552	40.921	5.800	1.00	18.60	CPS1
ATOM	46	CD2	LEU	7	57.546	40.825	7.342	1.00	19.42	CPS1
ATOM	47	C	LEU	7	58.025	44.246	4.780	1.00	18.80	CPS1
ATOM	48	O	LEU	7	57.036	44.935	4.988	1.00	19.60	CPS1
ATOM	49	N	ASP	8	58.240	43.632	3.623	1.00	18.18	CPS1
ATOM	50	CA	ASP	8	57.256	43.693	2.558	1.00	18.85	CPS1
ATOM	51	CB	ASP	8	57.514	44.898	1.629	1.00	20.11	CPS1
ATOM	52	CG	ASP	8	56.550	44.927	0.447	1.00	21.89	CPS1
ATOM	53	OD1	ASP	8	56.853	44.324	-0.600	1.00	24.47	CPS1
ATOM	54	OD2	ASP	8	55.471	45.524	0.585	1.00	25.95	CPS1
ATOM	55	C	ASP	8	57.293	42.422	1.723	1.00	18.97	CPS1
ATOM	56	O	ASP	8	58.353	41.856	1.486	1.00	19.21	CPS1

FIG. 1A-1

ATOM	57	N	ILE	9	56.124	41.944	1.328	1.00	19.03	CPS1
ATOM	58	CA	ILE	9	56.051	40.795	0.444	1.00	19.29	CPS1
ATOM	59	CB	ILE	9	55.393	39.567	1.093	1.00	21.16	CPS1
ATOM	60	CG2	ILE	9	55.354	38.416	0.080	1.00	20.76	CPS1
ATOM	61	CG1	ILE	9	56.198	39.115	2.308	1.00	19.57	CPS1
ATOM	62	CD1	ILE	9	55.560	37.946	3.081	1.00	21.48	CPS1
ATOM	63	C	ILE	9	55.161	41.304	-0.683	1.00	20.60	CPS1
ATOM	64	O	ILE	9	54.102	41.904	-0.431	1.00	18.57	CPS1
ATOM	65	N	THR	10	55.601	41.100	-1.916	1.00	20.85	CPS1
ATOM	66	CA	THR	10	54.828	41.556	-3.064	1.00	22.77	CPS1
ATOM	67	CB	THR	10	55.555	42.710	-3.789	1.00	25.32	CPS1
ATOM	68	OG1	THR	10	55.699	43.816	-2.889	1.00	26.50	CPS1
ATOM	69	CG2	THR	10	54.758	43.168	-5.014	1.00	26.33	CPS1
ATOM	70	C	THR	10	54.598	40.400	-4.028	1.00	22.74	CPS1
ATOM	71	O	THR	10	55.506	39.633	-4.314	1.00	21.67	CPS1
ATOM	72	N	GLU	11	53.359	40.270	-4.495	1.00	24.96	CPS1
ATOM	73	CA	GLU	11	52.993	39.223	-5.445	1.00	25.76	CPS1
ATOM	74	CB	GLU	11	51.475	38.995	-5.394	1.00	28.49	CPS1
ATOM	75	CG	GLU	11	50.969	37.968	-6.383	1.00	31.23	CPS1
ATOM	76	CD	GLU	11	49.445	37.895	-6.440	1.00	34.90	CPS1
ATOM	77	OE1	GLU	11	48.773	38.865	-6.019	1.00	33.91	CPS1
ATOM	78	OE2	GLU	11	48.923	36.867	-6.926	1.00	35.55	CPS1
ATOM	79	C	GLU	11	53.420	39.693	-6.842	1.00	25.44	CPS1
ATOM	80	O	GLU	11	53.000	40.761	-7.293	1.00	24.85	CPS1
ATOM	81	N	LEU	12	54.252	38.912	-7.525	1.00	26.00	CPS1
ATOM	82	CA	LEU	12	54.715	39.316	-8.857	1.00	27.71	CPS1
ATOM	83	CB	LEU	12	55.599	38.242	-9.488	1.00	28.64	CPS1
ATOM	84	CG	LEU	12	56.860	37.729	-8.793	1.00	31.06	CPS1
ATOM	85	CD1	LEU	12	57.721	37.022	-9.836	1.00	31.75	CPS1
ATOM	86	CD2	LEU	12	57.643	38.862	-8.157	1.00	31.13	CPS1
ATOM	87	C	LEU	12	53.557	39.608	-9.810	1.00	28.75	CPS1
ATOM	88	O	LEU	12	53.630	40.526	-10.631	1.00	28.32	CPS1
ATOM	89	N	ALA	13	52.498	38.813	-9.708	1.00	29.63	CPS1
ATOM	90	CA	ALA	13	51.330	38.987	-10.565	1.00	32.09	CPS1
ATOM	91	CB	ALA	13	50.281	37.918	-10.238	1.00	32.02	CPS1
ATOM	92	C	ALA	13	50.732	40.379	-10.397	1.00	33.63	CPS1
ATOM	93	O	ALA	13	50.280	41.000	-11.369	1.00	33.79	CPS1
ATOM	94	N	ARG	14	50.732	40.864	-9.160	1.00	34.46	CPS1
ATOM	95	CA	ARG	14	50.188	42.178	-8.846	1.00	35.63	CPS1
ATOM	96	CB	ARG	14	50.170	42.380	-7.330	1.00	38.10	CPS1
ATOM	97	CG	ARG	14	48.818	42.770	-6.772	1.00	41.02	CPS1
ATOM	98	CD	ARG	14	48.815	44.197	-6.276	1.00	42.88	CPS1
ATOM	99	NE	ARG	14	49.762	44.395	-5.183	1.00	43.99	CPS1
ATOM	100	CZ	ARG	14	50.030	45.575	-4.628	1.00	45.35	CPS1
ATOM	101	NH1	ARG	14	49.420	46.670	-5.063	1.00	46.27	CPS1
ATOM	102	NH2	ARG	14	50.915	45.664	-3.642	1.00	44.46	CPS1
ATOM	103	C	ARG	14	51.022	43.264	-9.508	1.00	36.31	CPS1
ATOM	104	O	ARG	14	50.484	44.232	-10.055	1.00	36.04	CPS1
ATOM	105	N	ILE	15	52.340	43.095	-9.457	1.00	35.62	CPS1
ATOM	106	CA	ILE	15	53.258	44.046	-10.062	1.00	36.49	CPS1
ATOM	107	CB	ILE	15	54.720	43.639	-9.788	1.00	34.84	CPS1
ATOM	108	CG2	ILE	15	55.666	44.453	-10.646	1.00	34.69	CPS1
ATOM	109	CG1	ILE	15	55.037	43.835	-8.298	1.00	32.18	CPS1
ATOM	110	CD1	ILE	15	54.936	45.275	-7.834	1.00	33.49	CPS1
ATOM	111	C	ILE	15	52.995	44.093	-11.566	1.00	39.03	CPS1
ATOM	112	O	ILE	15	53.103	45.147	-12.195	1.00	38.89	CPS1
ATOM	113	N	ALA	16	52.651	42.946	-12.141	1.00	41.54	CPS1

FIG. 1A-2

ATOM	114	CA	ALA	16	52.336	42.887	-13.564	1.00 44.64	CPS1
ATOM	115	CB	ALA	16	52.211	41.436	-14.018	1.00 44.42	CPS1
ATOM	116	C	ALA	16	51.016	43.629	-13.784	1.00 46.09	CPS1
ATOM	117	O	ALA	16	50.869	44.377	-14.746	1.00 47.05	CPS1
ATOM	118	N	SER	17	50.064	43.425	-12.877	1.00 49.05	CPS1
ATOM	119	CA	SER	17	48.752	44.076	-12.959	1.00 51.73	CPS1
ATOM	120	CB	SER	17	47.823	43.567	-11.851	1.00 51.91	CPS1
ATOM	121	OG	SER	17	47.472	42.208	-12.048	1.00 53.45	CPS1
ATOM	122	C	SER	17	48.851	45.594	-12.854	1.00 53.68	CPS1
ATOM	123	O	SER	17	48.310	46.316	-13.691	1.00 54.03	CPS1
ATOM	124	N	MET	18	49.530	46.075	-11.816	1.00 55.71	CPS1
ATOM	125	CA	MET	18	49.697	47.511	-11.611	1.00 57.69	CPS1
ATOM	126	CB	MET	18	50.429	47.787	-10.293	1.00 58.63	CPS1
ATOM	127	CG	MET	18	49.679	47.357	-9.046	1.00 60.86	CPS1
ATOM	128	SD	MET	18	50.678	47.547	-7.546	1.00 64.39	CPS1
ATOM	129	CE	MET	18	50.115	49.133	-6.944	1.00 63.23	CPS1
ATOM	130	C	MET	18	50.489	48.126	-12.758	1.00 58.14	CPS1
ATOM	131	O	MET	18	50.147	49.200	-13.253	1.00 58.47	CPS1
ATOM	132	N	ALA	19	51.545	47.440	-13.178	1.00 58.63	CPS1
ATOM	133	CA	ALA	19	52.393	47.930	-14.257	1.00 59.73	CPS1
ATOM	134	CB	ALA	19	53.432	46.881	-14.626	1.00 58.94	CPS1
ATOM	135	C	ALA	19	51.593	48.320	-15.490	1.00 61.14	CPS1
ATOM	136	O	ALA	19	51.267	49.491	-15.679	1.00 61.35	CPS1
ATOM	137	N	GLY	20	51.282	47.329	-16.322	1.00 62.81	CPS1
ATOM	138	CA	GLY	20	50.537	47.568	-17.549	1.00 64.34	CPS1
ATOM	139	C	GLY	20	49.331	48.486	-17.438	1.00 65.24	CPS1
ATOM	140	O	GLY	20	49.010	49.210	-18.382	1.00 65.67	CPS1
ATOM	141	N	ARG	21	48.660	48.459	-16.292	1.00 65.86	CPS1
ATOM	142	CA	ARG	21	47.485	49.295	-16.081	1.00 66.76	CPS1
ATOM	143	CB	ARG	21	46.595	48.672	-14.996	1.00 68.01	CPS1
ATOM	144	CG	ARG	21	45.294	49.417	-14.698	1.00 70.30	CPS1
ATOM	145	CD	ARG	21	44.482	49.731	-15.959	1.00 72.22	CPS1
ATOM	146	NE	ARG	21	44.987	50.908	-16.671	1.00 73.68	CPS1
ATOM	147	CZ	ARG	21	44.415	51.435	-17.750	1.00 74.14	CPS1
ATOM	148	NH1	ARG	21	43.314	50.891	-18.253	1.00 74.30	CPS1
ATOM	149	NH2	ARG	21	44.941	52.510	-18.324	1.00 74.39	CPS1
ATOM	150	C	ARG	21	47.862	50.728	-15.703	1.00 66.35	CPS1
ATOM	151	O	ARG	21	47.312	51.296	-14.759	1.00 66.83	CPS1
ATOM	152	N	GLN	22	48.803	51.304	-16.450	1.00 65.49	CPS1
ATOM	153	CA	GLN	22	49.263	52.676	-16.219	1.00 64.27	CPS1
ATOM	154	CB	GLN	22	50.068	52.755	-14.913	1.00 64.78	CPS1
ATOM	155	CG	GLN	22	49.187	52.941	-13.675	1.00 66.23	CPS1
ATOM	156	CD	GLN	22	49.924	52.717	-12.368	1.00 67.13	CPS1
ATOM	157	OE1	GLN	22	50.946	53.353	-12.097	1.00 67.87	CPS1
ATOM	158	NE2	GLN	22	49.401	51.812	-11.544	1.00 67.13	CPS1
ATOM	159	C	GLN	22	50.086	53.230	-17.393	1.00 62.83	CPS1
ATOM	160	O	GLN	22	49.559	53.962	-18.239	1.00 63.71	CPS1
ATOM	161	N	GLY	23	51.368	52.878	-17.452	1.00 59.93	CPS1
ATOM	162	CA	GLY	23	52.215	53.360	-18.532	1.00 54.65	CPS1
ATOM	163	C	GLY	23	53.259	54.325	-18.006	1.00 51.39	CPS1
ATOM	164	O	GLY	23	53.852	55.099	-18.765	1.00 50.70	CPS1
ATOM	165	N	ARG	24	53.474	54.268	-16.694	1.00 47.29	CPS1
ATOM	166	CA	ARG	24	54.433	55.121	-16.007	1.00 42.63	CPS1
ATOM	167	CB	ARG	24	53.798	56.490	-15.771	1.00 45.51	CPS1
ATOM	168	CG	ARG	24	54.684	57.512	-15.095	1.00 48.36	CPS1
ATOM	169	CD	ARG	24	54.194	58.925	-15.397	1.00 50.96	CPS1
ATOM	170	NE	ARG	24	52.773	59.092	-15.108	1.00 53.61	CPS1

FIG. 1A-3

ATOM	171	CZ	ARG	24	52.092	60.215	-15.320	1.00	54.82	CPS1
ATOM	172	NH1	ARG	24	52.704	61.281	-15.824	1.00	55.59	CPS1
ATOM	173	NH2	ARG	24	50.796	60.270	-15.039	1.00	55.48	CPS1
ATOM	174	C	ARG	24	54.842	54.480	-14.673	1.00	38.31	CPS1
ATOM	175	O	ARG	24	55.617	55.045	-13.906	1.00	35.06	CPS1
ATOM	176	N	PHE	25	54.338	53.279	-14.420	1.00	34.51	CPS1
ATOM	177	CA	PHE	25	54.630	52.585	-13.166	1.00	32.21	CPS1
ATOM	178	CB	PHE	25	53.805	51.298	-13.074	1.00	33.02	CPS1
ATOM	179	CG	PHE	25	54.016	50.536	-11.797	1.00	33.13	CPS1
ATOM	180	CD1	PHE	25	54.917	49.482	-11.741	1.00	33.65	CPS1
ATOM	181	CD2	PHE	25	53.323	50.889	-10.642	1.00	34.84	CPS1
ATOM	182	CE1	PHE	25	55.129	48.784	-10.553	1.00	33.64	CPS1
ATOM	183	CE2	PHE	25	53.527	50.201	-9.450	1.00	34.46	CPS1
ATOM	184	CZ	PHE	25	54.432	49.146	-9.405	1.00	34.16	CPS1
ATOM	185	C	PHE	25	56.103	52.273	-12.902	1.00	29.41	CPS1
ATOM	186	O	PHE	25	56.632	52.657	-11.862	1.00	29.18	CPS1
ATOM	187	N	ALA	26	56.771	51.585	-13.826	1.00	26.94	CPS1
ATOM	188	CA	ALA	26	58.177	51.245	-13.621	1.00	25.77	CPS1
ATOM	189	CB	ALA	26	58.702	50.403	-14.785	1.00	25.23	CPS1
ATOM	190	C	ALA	26	59.043	52.480	-13.459	1.00	25.39	CPS1
ATOM	191	O	ALA	26	59.955	52.511	-12.632	1.00	22.61	CPS1
ATOM	192	N	GLU	27	58.757	53.502	-14.260	1.00	24.05	CPS1
ATOM	193	CA	GLU	27	59.537	54.726	-14.210	1.00	25.73	CPS1
ATOM	194	CB	GLU	27	59.225	55.589	-15.436	1.00	25.99	CPS1
ATOM	195	CG	GLU	27	59.695	54.987	-16.750	1.00	26.79	CPS1
ATOM	196	CD	GLU	27	58.896	53.770	-17.202	1.00	28.20	CPS1
ATOM	197	OE1	GLU	27	57.680	53.695	-16.908	1.00	30.98	CPS1
ATOM	198	OE2	GLU	27	59.481	52.894	-17.877	1.00	29.45	CPS1
ATOM	199	C	GLU	27	59.315	55.519	-12.924	1.00	26.62	CPS1
ATOM	200	O	GLU	27	60.158	56.322	-12.532	1.00	27.44	CPS1
ATOM	201	N	ARG	28	58.179	55.312	-12.272	1.00	26.83	CPS1
ATOM	202	CA	ARG	28	57.924	56.002	-11.014	1.00	28.43	CPS1
ATOM	203	CB	ARG	28	56.422	56.062	-10.727	1.00	31.75	CPS1
ATOM	204	CG	ARG	28	55.736	57.322	-11.243	1.00	38.22	CPS1
ATOM	205	CD	ARG	28	54.229	57.195	-11.093	1.00	41.94	CPS1
ATOM	206	NE	ARG	28	53.891	56.446	-9.885	1.00	46.44	CPS1
ATOM	207	CZ	ARG	28	53.088	55.387	-9.869	1.00	47.55	CPS1
ATOM	208	NH1	ARG	28	52.534	54.953	-11.000	1.00	48.25	CPS1
ATOM	209	NH2	ARG	28	52.855	54.751	-8.726	1.00	49.13	CPS1
ATOM	210	C	ARG	28	58.629	55.267	-9.877	1.00	27.14	CPS1
ATOM	211	O	ARG	28	59.086	55.885	-8.928	1.00	27.28	CPS1
ATOM	212	N	ILE	29	58.729	53.944	-9.985	1.00	26.44	CPS1
ATOM	213	CA	ILE	29	59.363	53.137	-8.938	1.00	26.04	CPS1
ATOM	214	CB	ILE	29	58.901	51.657	-9.004	1.00	26.47	CPS1
ATOM	215	CG2	ILE	29	59.520	50.865	-7.858	1.00	28.14	CPS1
ATOM	216	CG1	ILE	29	57.374	51.565	-8.976	1.00	27.67	CPS1
ATOM	217	CD1	ILE	29	56.722	52.214	-7.796	1.00	28.72	CPS1
ATOM	218	C	ILE	29	60.888	53.122	-8.980	1.00	25.23	CPS1
ATOM	219	O	ILE	29	61.549	53.123	-7.934	1.00	25.57	CPS1
ATOM	220	N	LEU	30	61.445	53.119	-10.188	1.00	23.44	CPS1
ATOM	221	CA	LEU	30	62.885	53.031	-10.371	1.00	22.74	CPS1
ATOM	222	CB	LEU	30	63.185	52.029	-11.487	1.00	22.73	CPS1
ATOM	223	CG	LEU	30	62.509	50.656	-11.381	1.00	22.89	CPS1
ATOM	224	CD1	LEU	30	62.817	49.861	-12.635	1.00	22.68	CPS1
ATOM	225	CD2	LEU	30	63.004	49.922	-10.126	1.00	22.78	CPS1
ATOM	226	C	LEU	30	63.590	54.344	-10.686	1.00	23.94	CPS1
ATOM	227	O	LEU	30	63.027	55.228	-11.336	1.00	23.90	CPS1

FIG. 1A-4

ATOM	228	N	THR	31	64.830	54.451	-10.224	1.00 24.75	CPS1
ATOM	229	CA	THR	31	65.643	55.636	-10.461	1.00 25.03	CPS1
ATOM	230	CB	THR	31	66.787	55.749	-9.457	1.00 26.35	CPS1
ATOM	231	OG1	THR	31	67.725	54.692	-9.695	1.00 26.00	CPS1
ATOM	232	CG2	THR	31	66.261	55.671	-8.031	1.00 26.75	CPS1
ATOM	233	C	THR	31	66.271	55.469	-11.832	1.00 24.44	CPS1
ATOM	234	O	THR	31	66.163	54.416	-12.441	1.00 22.68	CPS1
ATOM	235	N	ARG	32	66.963	56.503	-12.293	1.00 25.91	CPS1
ATOM	236	CA	ARG	32	67.607	56.458	-13.603	1.00 26.68	CPS1
ATOM	237	CB	ARG	32	68.342	57.780	-13.848	1.00 26.75	CPS1
ATOM	238	CG	ARG	32	68.970	57.939	-15.236	1.00 29.21	CPS1
ATOM	239	CD	ARG	32	69.551	59.348	-15.344	1.00 29.81	CPS1
ATOM	240	NE	ARG	32	70.015	59.707	-16.684	1.00 32.75	CPS1
ATOM	241	CZ	ARG	32	71.129	59.256	-17.254	1.00 34.02	CPS1
ATOM	242	NH1	ARG	32	71.916	58.404	-16.606	1.00 33.55	CPS1
ATOM	243	NH2	ARG	32	71.476	59.692	-18.464	1.00 31.94	CPS1
ATOM	244	C	ARG	32	68.572	55.276	-13.728	1.00 26.02	CPS1
ATOM	245	O	ARG	32	68.539	54.542	-14.721	1.00 25.46	CPS1
ATOM	246	N	SER	33	69.422	55.088	-12.721	1.00 26.77	CPS1
ATOM	247	CA	SER	33	70.390	53.990	-12.725	1.00 28.08	CPS1
ATOM	248	CB	SER	33	71.277	54.037	-11.473	1.00 31.22	CPS1
ATOM	249	OG	SER	33	72.112	55.182	-11.481	1.00 38.13	CPS1
ATOM	250	C	SER	33	69.686	52.645	-12.772	1.00 27.50	CPS1
ATOM	251	O	SER	33	70.113	51.738	-13.487	1.00 28.27	CPS1
ATOM	252	N	GLU	34	68.613	52.510	-11.998	1.00 25.55	CPS1
ATOM	253	CA	GLU	34	67.857	51.262	-11.970	1.00 25.24	CPS1
ATOM	254	CB	GLU	34	66.842	51.298	-10.822	1.00 25.04	CPS1
ATOM	255	CG	GLU	34	67.531	51.247	-9.455	1.00 24.32	CPS1
ATOM	256	CD	GLU	34	66.575	51.424	-8.280	1.00 26.32	CPS1
ATOM	257	OE1	GLU	34	66.860	50.849	-7.202	1.00 24.86	CPS1
ATOM	258	OE2	GLU	34	65.557	52.145	-8.423	1.00 25.42	CPS1
ATOM	259	C	GLU	34	67.167	50.997	-13.302	1.00 25.57	CPS1
ATOM	260	O	GLU	34	67.113	49.852	-13.767	1.00 26.12	CPS1
ATOM	261	N	LEU	35	66.649	52.056	-13.919	1.00 25.65	CPS1
ATOM	262	CA	LEU	35	65.978	51.931	-15.209	1.00 25.43	CPS1
ATOM	263	CB	LEU	35	65.362	53.269	-15.626	1.00 24.81	CPS1
ATOM	264	CG	LEU	35	64.044	53.625	-14.936	1.00 25.80	CPS1
ATOM	265	CD1	LEU	35	63.598	55.028	-15.354	1.00 24.72	CPS1
ATOM	266	CD2	LEU	35	62.980	52.592	-15.320	1.00 24.55	CPS1
ATOM	267	C	LEU	35	66.961	51.465	-16.278	1.00 25.60	CPS1
ATOM	268	O	LEU	35	66.608	50.663	-17.139	1.00 25.96	CPS1
ATOM	269	N	ASP	36	68.189	51.968	-16.213	1.00 26.39	CPS1
ATOM	270	CA	ASP	36	69.221	51.586	-17.176	1.00 28.65	CPS1
ATOM	271	CB	ASP	36	70.549	52.267	-16.814	1.00 30.67	CPS1
ATOM	272	CG	ASP	36	71.653	51.992	-17.834	1.00 34.97	CPS1
ATOM	273	OD1	ASP	36	71.397	52.122	-19.045	1.00 36.35	CPS1
ATOM	274	OD2	ASP	36	72.780	51.653	-17.421	1.00 38.35	CPS1
ATOM	275	C	ASP	36	69.374	50.061	-17.176	1.00 29.59	CPS1
ATOM	276	O	ASP	36	69.510	49.429	-18.229	1.00 29.62	CPS1
ATOM	277	N	GLN	37	69.331	49.466	-15.987	1.00 29.16	CPS1
ATOM	278	CA	GLN	37	69.446	48.019	-15.860	1.00 27.84	CPS1
ATOM	279	CB	GLN	37	69.737	47.648	-14.404	1.00 29.01	CPS1
ATOM	280	CG	GLN	37	70.983	48.305	-13.850	1.00 32.00	CPS1
ATOM	281	CD	GLN	37	71.075	48.186	-12.348	1.00 34.39	CPS1
ATOM	282	OE1	GLN	37	71.087	47.079	-11.805	1.00 34.90	CPS1
ATOM	283	NE2	GLN	37	71.142	49.329	-11.662	1.00 34.48	CPS1
ATOM	284	C	GLN	37	68.156	47.335	-16.301	1.00 27.75	CPS1

FIG. 1A-5

ATOM	285	O	GLN	37	68.183	46.328	-17.012	1.00 27.75	CPS1
ATOM	286	N	TYR	38	67.031	47.885	-15.858	1.00 26.28	CPS1
ATOM	287	CA	TYR	38	65.705	47.352	-16.167	1.00 25.28	CPS1
ATOM	288	CB	TYR	38	64.657	48.251	-15.500	1.00 25.99	CPS1
ATOM	289	CG	TYR	38	63.213	47.908	-15.772	1.00 26.20	CPS1
ATOM	290	CD1	TYR	38	62.468	48.648	-16.688	1.00 26.19	CPS1
ATOM	291	CE1	TYR	38	61.121	48.385	-16.903	1.00 26.29	CPS1
ATOM	292	CD2	TYR	38	62.567	46.881	-15.074	1.00 26.31	CPS1
ATOM	293	CE2	TYR	38	61.219	46.611	-15.280	1.00 25.67	CPS1
ATOM	294	CZ	TYR	38	60.501	47.370	-16.200	1.00 28.03	CPS1
ATOM	295	OH	TYR	38	59.166	47.120	-16.428	1.00 27.03	CPS1
ATOM	296	C	TYR	38	65.420	47.208	-17.668	1.00 26.52	CPS1
ATOM	297	O	TYR	38	64.912	46.175	-18.122	1.00 23.95	CPS1
ATOM	298	N	TYR	39	65.756	48.235	-18.440	1.00 26.98	CPS1
ATOM	299	CA	TYR	39	65.502	48.193	-19.880	1.00 29.18	CPS1
ATOM	300	CB	TYR	39	65.757	49.579	-20.488	1.00 28.06	CPS1
ATOM	301	CG	TYR	39	64.725	50.615	-20.060	1.00 27.09	CPS1
ATOM	302	CD1	TYR	39	63.365	50.313	-20.080	1.00 26.88	CPS1
ATOM	303	CE1	TYR	39	62.402	51.252	-19.691	1.00 26.96	CPS1
ATOM	304	CD2	TYR	39	65.109	51.890	-19.641	1.00 26.42	CPS1
ATOM	305	CE2	TYR	39	64.154	52.841	-19.245	1.00 27.05	CPS1
ATOM	306	CZ	TYR	39	62.806	52.510	-19.274	1.00 26.67	CPS1
ATOM	307	OH	TYR	39	61.856	53.426	-18.876	1.00 27.91	CPS1
ATOM	308	C	TYR	39	66.279	47.108	-20.641	1.00 31.26	CPS1
ATOM	309	O	TYR	39	65.899	46.727	-21.750	1.00 32.43	CPS1
ATOM	310	N	GLU	40	67.351	46.597	-20.046	1.00 32.52	CPS1
ATOM	311	CA	GLU	40	68.150	45.555	-20.690	1.00 33.92	CPS1
ATOM	312	CB	GLU	40	69.602	45.621	-20.207	1.00 35.68	CPS1
ATOM	313	CG	GLU	40	70.340	46.890	-20.579	1.00 38.76	CPS1
ATOM	314	CD	GLU	40	70.370	47.130	-22.079	1.00 41.13	CPS1
ATOM	315	OE1	GLU	40	70.557	46.153	-22.835	1.00 43.88	CPS1
ATOM	316	OE2	GLU	40	70.220	48.297	-22.501	1.00 41.69	CPS1
ATOM	317	C	GLU	40	67.616	44.147	-20.419	1.00 34.35	CPS1
ATOM	318	O	GLU	40	68.089	43.177	-21.008	1.00 33.76	CPS1
ATOM	319	N	LEU	41	66.626	44.036	-19.541	1.00 33.60	CPS1
ATOM	320	CA	LEU	41	66.080	42.733	-19.176	1.00 34.81	CPS1
ATOM	321	CB	LEU	41	65.658	42.757	-17.702	1.00 33.78	CPS1
ATOM	322	CG	LEU	41	66.725	43.183	-16.690	1.00 33.47	CPS1
ATOM	323	CD1	LEU	41	66.084	43.291	-15.309	1.00 33.49	CPS1
ATOM	324	CD2	LEU	41	67.879	42.188	-16.678	1.00 33.26	CPS1
ATOM	325	C	LEU	41	64.910	42.221	-20.013	1.00 35.00	CPS1
ATOM	326	O	LEU	41	64.199	42.992	-20.654	1.00 34.86	CPS1
ATOM	327	N	SER	42	64.713	40.904	-19.984	1.00 36.21	CPS1
ATOM	328	CA	SER	42	63.615	40.271	-20.709	1.00 37.02	CPS1
ATOM	329	CB	SER	42	63.788	38.752	-20.716	1.00 37.19	CPS1
ATOM	330	OG	SER	42	63.601	38.228	-19.413	1.00 37.95	CPS1
ATOM	331	C	SER	42	62.321	40.628	-19.986	1.00 37.67	CPS1
ATOM	332	O	SER	42	62.355	41.124	-18.856	1.00 37.09	CPS1
ATOM	333	N	GLU	43	61.180	40.378	-20.618	1.00 37.74	CPS1
ATOM	334	CA	GLU	43	59.917	40.705	-19.970	1.00 39.67	CPS1
ATOM	335	CB	GLU	43	58.716	40.282	-20.829	1.00 42.30	CPS1
ATOM	336	CG	GLU	43	57.421	40.990	-20.417	1.00 46.74	CPS1
ATOM	337	CD	GLU	43	56.177	40.466	-21.122	1.00 49.57	CPS1
ATOM	338	OE1	GLU	43	56.253	40.155	-22.333	1.00 51.74	CPS1
ATOM	339	OE2	GLU	43	55.116	40.384	-20.465	1.00 50.82	CPS1
ATOM	340	C	GLU	43	59.833	40.012	-18.611	1.00 38.42	CPS1
ATOM	341	O	GLU	43	59.425	40.619	-17.623	1.00 37.06	CPS1

FIG. 1A-6

ATOM	342	N	LYS	44	60.223	38.743	-18.567	1.00 37.89	CPS1
ATOM	343	CA	LYS	44	60.176	37.985	-17.318	1.00 38.86	CPS1
ATOM	344	CB	LYS	44	60.566	36.525	-17.562	1.00 40.32	CPS1
ATOM	345	CG	LYS	44	60.777	35.706	-16.292	1.00 43.45	CPS1
ATOM	346	CD	LYS	44	60.766	34.214	-16.594	1.00 46.17	CPS1
ATOM	347	CE	LYS	44	61.613	33.425	-15.603	1.00 47.94	CPS1
ATOM	348	NZ	LYS	44	63.073	33.691	-15.805	1.00 50.56	CPS1
ATOM	349	C	LYS	44	61.086	38.587	-16.257	1.00 37.33	CPS1
ATOM	350	O	LYS	44	60.661	38.823	-15.127	1.00 36.33	CPS1
ATOM	351	N	ARG	45	62.338	38.835	-16.625	1.00 36.56	CPS1
ATOM	352	CA	ARG	45	63.310	39.403	-15.695	1.00 35.88	CPS1
ATOM	353	CB	ARG	45	64.700	39.412	-16.333	1.00 37.23	CPS1
ATOM	354	CG	ARG	45	65.356	38.041	-16.385	1.00 39.66	CPS1
ATOM	355	CD	ARG	45	65.840	37.633	-15.008	1.00 42.70	CPS1
ATOM	356	NE	ARG	45	66.842	38.569	-14.498	1.00 45.11	CPS1
ATOM	357	CZ	ARG	45	66.700	39.307	-13.399	1.00 46.10	CPS1
ATOM	358	NH1	ARG	45	65.593	39.226	-12.672	1.00 45.56	CPS1
ATOM	359	NH2	ARG	45	67.666	40.140	-13.033	1.00 47.39	CPS1
ATOM	360	C	ARG	45	62.920	40.807	-15.254	1.00 34.51	CPS1
ATOM	361	O	ARG	45	63.182	41.200	-14.120	1.00 33.99	CPS1
ATOM	362	N	LYS	46	62.294	41.565	-16.148	1.00 32.94	CPS1
ATOM	363	CA	LYS	46	61.857	42.911	-15.802	1.00 32.28	CPS1
ATOM	364	CB	LYS	46	61.165	43.580	-16.990	1.00 32.34	CPS1
ATOM	365	CG	LYS	46	62.109	44.110	-18.051	1.00 32.52	CPS1
ATOM	366	CD	LYS	46	61.327	44.905	-19.113	1.00 33.61	CPS1
ATOM	367	CE	LYS	46	62.262	45.515	-20.151	1.00 34.98	CPS1
ATOM	368	NZ	LYS	46	61.505	46.250	-21.211	1.00 36.94	CPS1
ATOM	369	C	LYS	46	60.888	42.868	-14.621	1.00 31.45	CPS1
ATOM	370	O	LYS	46	61.002	43.655	-13.684	1.00 30.01	CPS1
ATOM	371	N	ASN	47	59.937	41.942	-14.672	1.00 30.18	CPS1
ATOM	372	CA	ASN	47	58.951	41.806	-13.606	1.00 30.39	CPS1
ATOM	373	CB	ASN	47	57.886	40.773	-14.012	1.00 32.50	CPS1
ATOM	374	CG	ASN	47	56.914	40.449	-12.885	1.00 35.59	CPS1
ATOM	375	OD1	ASN	47	57.020	39.401	-12.246	1.00 39.44	CPS1
ATOM	376	ND2	ASN	47	55.969	41.346	-12.635	1.00 35.35	CPS1
ATOM	377	C	ASN	47	59.608	41.424	-12.273	1.00 28.81	CPS1
ATOM	378	O	ASN	47	59.252	41.971	-11.230	1.00 27.56	CPS1
ATOM	379	N	GLU	48	60.568	40.503	-12.308	1.00 27.77	CPS1
ATOM	380	CA	GLU	48	61.265	40.064	-11.093	1.00 26.38	CPS1
ATOM	381	CB	GLU	48	62.172	38.870	-11.417	1.00 30.74	CPS1
ATOM	382	CG	GLU	48	61.417	37.675	-12.004	1.00 34.10	CPS1
ATOM	383	CD	GLU	48	62.338	36.589	-12.553	1.00 37.43	CPS1
ATOM	384	OE1	GLU	48	61.815	35.595	-13.106	1.00 38.39	CPS1
ATOM	385	OE2	GLU	48	63.577	36.727	-12.434	1.00 38.18	CPS1
ATOM	386	C	GLU	48	62.101	41.201	-10.498	1.00 26.11	CPS1
ATOM	387	O	GLU	48	62.132	41.416	-9.271	1.00 22.48	CPS1
ATOM	388	N	PHE	49	62.792	41.919	-11.377	1.00 23.64	CPS1
ATOM	389	CA	PHE	49	63.628	43.042	-10.976	1.00 24.48	CPS1
ATOM	390	CB	PHE	49	64.356	43.591	-12.197	1.00 24.05	CPS1
ATOM	391	CG	PHE	49	65.252	44.754	-11.903	1.00 24.66	CPS1
ATOM	392	CD1	PHE	49	66.591	44.552	-11.572	1.00 26.69	CPS1
ATOM	393	CD2	PHE	49	64.771	46.052	-11.982	1.00 23.63	CPS1
ATOM	394	CE1	PHE	49	67.438	45.632	-11.329	1.00 27.13	CPS1
ATOM	395	CE2	PHE	49	65.601	47.137	-11.743	1.00 25.03	CPS1
ATOM	396	CZ	PHE	49	66.938	46.933	-11.416	1.00 26.71	CPS1
ATOM	397	C	PHE	49	62.777	44.152	-10.364	1.00 23.89	CPS1
ATOM	398	O	PHE	49	63.124	44.721	-9.323	1.00 24.30	CPS1

FIG. 1A-7

ATOM	399	N	LEU	50	61.672	44.476	-11.029	1.00	22.90	CPS1
ATOM	400	CA	LEU	50	60.795	45.534	-10.557	1.00	23.71	CPS1
ATOM	401	CB	LEU	50	59.732	45.836	-11.617	1.00	24.35	CPS1
ATOM	402	CG	LEU	50	58.714	46.928	-11.325	1.00	25.33	CPS1
ATOM	403	CD1	LEU	50	59.403	48.253	-11.010	1.00	24.88	CPS1
ATOM	404	CD2	LEU	50	57.805	47.055	-12.536	1.00	25.38	CPS1
ATOM	405	C	LEU	50	60.132	45.138	-9.236	1.00	23.44	CPS1
ATOM	406	O	LEU	50	60.011	45.957	-8.322	1.00	22.54	CPS1
ATOM	407	N	ALA	51	59.698	43.884	-9.148	1.00	22.99	CPS1
ATOM	408	CA	ALA	51	59.056	43.399	-7.929	1.00	23.20	CPS1
ATOM	409	CB	ALA	51	58.581	41.959	-8.123	1.00	23.60	CPS1
ATOM	410	C	ALA	51	60.034	43.476	-6.754	1.00	21.98	CPS1
ATOM	411	O	ALA	51	59.655	43.884	-5.653	1.00	23.47	CPS1
ATOM	412	N	GLY	52	61.284	43.089	-6.998	1.00	21.48	CPS1
ATOM	413	CA	GLY	52	62.297	43.120	-5.951	1.00	22.37	CPS1
ATOM	414	C	GLY	52	62.585	44.523	-5.460	1.00	22.17	CPS1
ATOM	415	O	GLY	52	62.715	44.764	-4.256	1.00	21.91	CPS1
ATOM	416	N	ARG	53	62.675	45.461	-6.402	1.00	23.24	CPS1
ATOM	417	CA	ARG	53	62.933	46.862	-6.076	1.00	23.63	CPS1
ATOM	418	CB	ARG	53	63.169	47.654	-7.364	1.00	25.69	CPS1
ATOM	419	CG	ARG	53	64.546	48.242	-7.490	1.00	29.63	CPS1
ATOM	420	CD	ARG	53	65.618	47.212	-7.338	1.00	28.33	CPS1
ATOM	421	NE	ARG	53	66.937	47.751	-7.675	1.00	29.58	CPS1
ATOM	422	CZ	ARG	53	67.976	46.986	-7.980	1.00	29.37	CPS1
ATOM	423	NH1	ARG	53	67.821	45.670	-7.978	1.00	29.23	CPS1
ATOM	424	NH2	ARG	53	69.153	47.525	-8.299	1.00	26.48	CPS1
ATOM	425	C	ARG	53	61.752	47.468	-5.336	1.00	23.34	CPS1
ATOM	426	O	ARG	53	61.921	48.237	-4.389	1.00	22.79	CPS1
ATOM	427	N	PHE	54	60.551	47.146	-5.801	1.00	22.67	CPS1
ATOM	428	CA	PHE	54	59.335	47.638	-5.181	1.00	22.96	CPS1
ATOM	429	CB	PHE	54	58.114	47.106	-5.947	1.00	22.72	CPS1
ATOM	430	CG	PHE	54	56.807	47.619	-5.429	1.00	24.49	CPS1
ATOM	431	CD1	PHE	54	56.074	46.882	-4.506	1.00	24.85	CPS1
ATOM	432	CD2	PHE	54	56.329	48.865	-5.828	1.00	24.29	CPS1
ATOM	433	CE1	PHE	54	54.883	47.376	-3.983	1.00	25.96	CPS1
ATOM	434	CE2	PHE	54	55.143	49.370	-5.316	1.00	25.86	CPS1
ATOM	435	CZ	PHE	54	54.414	48.624	-4.387	1.00	26.67	CPS1
ATOM	436	C	PHE	54	59.285	47.177	-3.724	1.00	22.66	CPS1
ATOM	437	O	PHE	54	59.018	47.970	-2.808	1.00	21.27	CPS1
ATOM	438	N	ALA	55	59.556	45.896	-3.508	1.00	20.95	CPS1
ATOM	439	CA	ALA	55	59.524	45.349	-2.147	1.00	20.91	CPS1
ATOM	440	CB	ALA	55	59.733	43.846	-2.191	1.00	20.44	CPS1
ATOM	441	C	ALA	55	60.568	45.990	-1.234	1.00	20.32	CPS1
ATOM	442	O	ALA	55	60.288	46.295	-0.075	1.00	18.66	CPS1
ATOM	443	N	ALA	56	61.779	46.172	-1.751	1.00	18.74	CPS1
ATOM	444	CA	ALA	56	62.861	46.761	-0.971	1.00	19.35	CPS1
ATOM	445	CB	ALA	56	64.180	46.698	-1.762	1.00	19.52	CPS1
ATOM	446	C	ALA	56	62.543	48.201	-0.593	1.00	20.45	CPS1
ATOM	447	O	ALA	56	62.773	48.617	0.543	1.00	18.52	CPS1
ATOM	448	N	LYS	57	62.015	48.969	-1.545	1.00	18.95	CPS1
ATOM	449	CA	LYS	57	61.677	50.352	-1.270	1.00	19.87	CPS1
ATOM	450	CB	LYS	57	61.427	51.107	-2.583	1.00	19.77	CPS1
ATOM	451	CG	LYS	57	62.707	51.225	-3.393	1.00	20.64	CPS1
ATOM	452	CD	LYS	57	62.533	52.055	-4.679	1.00	21.45	CPS1
ATOM	453	CE	LYS	57	63.801	51.995	-5.512	1.00	22.31	CPS1
ATOM	454	NZ	LYS	57	63.888	53.112	-6.510	1.00	22.70	CPS1
ATOM	455	C	LYS	57	60.487	50.461	-0.329	1.00	19.95	CPS1

FIG. 1A-8

ATOM	456	O	LYS	57	60.458	51.352	0.515	1.00	20.79	CPS1
ATOM	457	N	GLU	58	59.513	49.561	-0.463	1.00	19.28	CPS1
ATOM	458	CA	GLU	58	58.358	49.567	0.436	1.00	21.04	CPS1
ATOM	459	CB	GLU	58	57.324	48.516	0.013	1.00	22.82	CPS1
ATOM	460	CG	GLU	58	56.428	48.907	-1.170	1.00	28.45	CPS1
ATOM	461	CD	GLU	58	55.586	50.145	-0.886	1.00	31.31	CPS1
ATOM	462	OE1	GLU	58	55.244	50.371	0.295	1.00	33.36	CPS1
ATOM	463	OE2	GLU	58	55.253	50.886	-1.840	1.00	34.15	CPS1
ATOM	464	C	GLU	58	58.851	49.242	1.856	1.00	19.94	CPS1
ATOM	465	O	GLU	58	58.456	49.899	2.818	1.00	19.84	CPS1
ATOM	466	N	ALA	59	59.717	48.234	1.979	1.00	18.95	CPS1
ATOM	467	CA	ALA	59	60.251	47.861	3.300	1.00	19.85	CPS1
ATOM	468	CB	ALA	59	61.155	46.618	3.185	1.00	18.19	CPS1
ATOM	469	C	ALA	59	61.044	49.037	3.881	1.00	20.46	CPS1
ATOM	470	O	ALA	59	60.954	49.359	5.076	1.00	20.70	CPS1
ATOM	471	N	PHE	60	61.831	49.691	3.042	1.00	19.23	CPS1
ATOM	472	CA	PHE	60	62.606	50.824	3.538	1.00	19.91	CPS1
ATOM	473	CB	PHE	60	63.500	51.407	2.440	1.00	20.97	CPS1
ATOM	474	CG	PHE	60	64.280	52.613	2.893	1.00	21.48	CPS1
ATOM	475	CD1	PHE	60	65.503	52.463	3.530	1.00	21.47	CPS1
ATOM	476	CD2	PHE	60	63.737	53.891	2.768	1.00	23.08	CPS1
ATOM	477	CE1	PHE	60	66.183	53.576	4.053	1.00	22.10	CPS1
ATOM	478	CE2	PHE	60	64.403	55.017	3.286	1.00	23.29	CPS1
ATOM	479	CZ	PHE	60	65.628	54.852	3.930	1.00	23.90	CPS1
ATOM	480	C	PHE	60	61.673	51.919	4.047	1.00	20.74	CPS1
ATOM	481	O	PHE	60	61.916	52.515	5.098	1.00	21.03	CPS1
ATOM	482	N	SER	61	60.604	52.191	3.302	1.00	20.69	CPS1
ATOM	483	CA	SER	61	59.669	53.237	3.702	1.00	21.92	CPS1
ATOM	484	CB	SER	61	58.625	53.488	2.607	1.00	22.10	CPS1
ATOM	485	OG	SER	61	57.716	52.406	2.499	1.00	23.85	CPS1
ATOM	486	C	SER	61	58.967	52.917	5.020	1.00	22.52	CPS1
ATOM	487	O	SER	61	58.574	53.824	5.760	1.00	23.57	CPS1
ATOM	488	N	LYS	62	58.811	51.633	5.314	1.00	21.64	CPS1
ATOM	489	CA	LYS	62	58.170	51.220	6.563	1.00	22.44	CPS1
ATOM	490	CB	LYS	62	57.705	49.767	6.463	1.00	22.20	CPS1
ATOM	491	CG	LYS	62	56.539	49.575	5.483	1.00	25.33	CPS1
ATOM	492	CD	LYS	62	56.149	48.113	5.354	1.00	29.01	CPS1
ATOM	493	CE	LYS	62	54.862	47.975	4.560	1.00	32.68	CPS1
ATOM	494	NZ	LYS	62	54.355	46.585	4.526	1.00	36.07	CPS1
ATOM	495	C	LYS	62	59.155	51.392	7.719	1.00	22.39	CPS1
ATOM	496	O	LYS	62	58.782	51.841	8.806	1.00	21.87	CPS1
ATOM	497	N	ALA	63	60.413	51.040	7.479	1.00	20.82	CPS1
ATOM	498	CA	ALA	63	61.444	51.194	8.502	1.00	21.70	CPS1
ATOM	499	CB	ALA	63	62.755	50.574	8.022	1.00	22.55	CPS1
ATOM	500	C	ALA	63	61.633	52.688	8.786	1.00	23.41	CPS1
ATOM	501	O	ALA	63	61.886	53.092	9.928	1.00	22.35	CPS1
ATOM	502	N	PHE	64	61.498	53.498	7.737	1.00	23.23	CPS1
ATOM	503	CA	PHE	64	61.638	54.946	7.838	1.00	25.59	CPS1
ATOM	504	CB	PHE	64	61.638	55.559	6.430	1.00	27.30	CPS1
ATOM	505	CG	PHE	64	62.121	56.979	6.381	1.00	30.46	CPS1
ATOM	506	CD1	PHE	64	63.464	57.279	6.593	1.00	31.49	CPS1
ATOM	507	CD2	PHE	64	61.237	58.015	6.107	1.00	29.70	CPS1
ATOM	508	CE1	PHE	64	63.920	58.596	6.528	1.00	33.53	CPS1
ATOM	509	CE2	PHE	64	61.681	59.333	6.039	1.00	31.57	CPS1
ATOM	510	CZ	PHE	64	63.021	59.624	6.249	1.00	32.65	CPS1
ATOM	511	C	PHE	64	60.477	55.504	8.667	1.00	26.41	CPS1
ATOM	512	O	PHE	64	60.564	56.613	9.193	1.00	27.04	CPS1

FIG. 1A-9

ATOM	513	N	GLY	65	59.388	54.735	8.751	1.00	27.22	CPS1
ATOM	514	CA	GLY	65	58.229	55.102	9.554	1.00	28.06	CPS1
ATOM	515	C	GLY	65	57.135	55.940	8.923	1.00	29.26	CPS1
ATOM	516	O	GLY	65	56.143	56.260	9.577	1.00	29.04	CPS1
ATOM	517	N	THR	66	57.299	56.279	7.650	1.00	29.45	CPS1
ATOM	518	CA	THR	66	56.333	57.119	6.951	1.00	30.32	CPS1
ATOM	519	CB	THR	66	57.033	58.351	6.391	1.00	30.19	CPS1
ATOM	520	OG1	THR	66	57.997	57.922	5.424	1.00	31.68	CPS1
ATOM	521	CG2	THR	66	57.751	59.114	7.489	1.00	31.63	CPS1
ATOM	522	C	THR	66	55.640	56.453	5.764	1.00	30.61	CPS1
ATOM	523	O	THR	66	54.548	56.862	5.365	1.00	30.50	CPS1
ATOM	524	N	GLY	67	56.280	55.443	5.188	1.00	30.12	CPS1
ATOM	525	CA	GLY	67	55.713	54.809	4.011	1.00	30.43	CPS1
ATOM	526	C	GLY	67	56.020	55.750	2.852	1.00	31.44	CPS1
ATOM	527	O	GLY	67	56.622	56.806	3.058	1.00	30.31	CPS1
ATOM	528	N	ILE	68	55.626	55.383	1.639	1.00	31.40	CPS1
ATOM	529	CA	ILE	68	55.886	56.239	0.486	1.00	32.28	CPS1
ATOM	530	CB	ILE	68	55.869	55.429	-0.844	1.00	31.80	CPS1
ATOM	531	CG2	ILE	68	56.083	56.375	-2.048	1.00	32.06	CPS1
ATOM	532	CG1	ILE	68	56.975	54.364	-0.826	1.00	29.99	CPS1
ATOM	533	CD1	ILE	68	58.391	54.924	-0.821	1.00	29.70	CPS1
ATOM	534	C	ILE	68	54.812	57.315	0.429	1.00	33.69	CPS1
ATOM	535	O	ILE	68	53.623	57.028	0.556	1.00	34.51	CPS1
ATOM	536	N	GLY	69	55.233	58.558	0.248	1.00	35.19	CPS1
ATOM	537	CA	GLY	69	54.281	59.649	0.187	1.00	36.88	CPS1
ATOM	538	C	GLY	69	54.989	60.985	0.167	1.00	37.34	CPS1
ATOM	539	O	GLY	69	56.065	61.115	-0.413	1.00	37.87	CPS1
ATOM	540	N	ALA	70	54.394	61.977	0.821	1.00	38.19	CPS1
ATOM	541	CA	ALA	70	54.964	63.314	0.866	1.00	38.33	CPS1
ATOM	542	CB	ALA	70	54.010	64.252	1.609	1.00	39.53	CPS1
ATOM	543	C	ALA	70	56.352	63.383	1.493	1.00	38.24	CPS1
ATOM	544	O	ALA	70	57.188	64.171	1.067	1.00	39.11	CPS1
ATOM	545	N	GLN	71	56.612	62.547	2.494	1.00	38.21	CPS1
ATOM	546	CA	GLN	71	57.901	62.578	3.177	1.00	37.58	CPS1
ATOM	547	CB	GLN	71	57.704	62.177	4.642	1.00	40.14	CPS1
ATOM	548	CG	GLN	71	56.511	62.867	5.297	1.00	44.12	CPS1
ATOM	549	CD	GLN	71	56.276	62.410	6.724	1.00	45.82	CPS1
ATOM	550	OE1	GLN	71	57.140	62.570	7.587	1.00	46.65	CPS1
ATOM	551	NE2	GLN	71	55.101	61.838	6.980	1.00	46.84	CPS1
ATOM	552	C	GLN	71	58.997	61.706	2.557	1.00	35.81	CPS1
ATOM	553	O	GLN	71	60.175	61.854	2.885	1.00	35.04	CPS1
ATOM	554	N	LEU	72	58.619	60.805	1.662	1.00	33.50	CPS1
ATOM	555	CA	LEU	72	59.602	59.917	1.053	1.00	31.98	CPS1
ATOM	556	CB	LEU	72	59.899	58.762	2.010	1.00	30.93	CPS1
ATOM	557	CG	LEU	72	60.905	57.699	1.561	1.00	30.26	CPS1
ATOM	558	CD1	LEU	72	62.311	58.276	1.592	1.00	31.32	CPS1
ATOM	559	CD2	LEU	72	60.801	56.483	2.490	1.00	29.64	CPS1
ATOM	560	C	LEU	72	59.104	59.364	-0.269	1.00	30.33	CPS1
ATOM	561	O	LEU	72	58.025	58.794	-0.333	1.00	30.73	CPS1
ATOM	562	N	SER	73	59.907	59.526	-1.315	1.00	30.09	CPS1
ATOM	563	CA	SER	73	59.550	59.051	-2.649	1.00	30.01	CPS1
ATOM	564	CB	SER	73	59.795	60.161	-3.679	1.00	30.79	CPS1
ATOM	565	OG	SER	73	59.700	59.659	-5.007	1.00	33.48	CPS1
ATOM	566	C	SER	73	60.348	57.824	-3.070	1.00	28.08	CPS1
ATOM	567	O	SER	73	61.447	57.596	-2.574	1.00	28.49	CPS1
ATOM	568	N	PHE	74	59.792	57.032	-3.985	1.00	28.86	CPS1
ATOM	569	CA	PHE	74	60.512	55.869	-4.502	1.00	28.18	CPS1

FIG. 1A-10

ATOM	570	CB	PHE	74	59.712	55.173	-5.608	1.00	28.46	CPS1
ATOM	571	CG	PHE	74	58.581	54.331	-5.106	1.00	28.51	CPS1
ATOM	572	CD1	PHE	74	58.833	53.164	-4.398	1.00	29.22	CPS1
ATOM	573	CD2	PHE	74	57.264	54.695	-5.358	1.00	28.56	CPS1
ATOM	574	CE1	PHE	74	57.789	52.364	-3.951	1.00	29.35	CPS1
ATOM	575	CE2	PHE	74	56.213	53.907	-4.914	1.00	30.56	CPS1
ATOM	576	CZ	PHE	74	56.479	52.734	-4.209	1.00	28.99	CPS1
ATOM	577	C	PHE	74	61.818	56.377	-5.107	1.00	29.02	CPS1
ATOM	578	O	PHE	74	62.846	55.697	-5.076	1.00	28.52	CPS1
ATOM	579	N	GLN	75	61.776	57.586	-5.660	1.00	29.54	CPS1
ATOM	580	CA	GLN	75	62.959	58.168	-6.289	1.00	30.04	CPS1
ATOM	581	CB	GLN	75	62.555	59.395	-7.117	1.00	31.75	CPS1
ATOM	582	CG	GLN	75	61.636	59.056	-8.284	1.00	31.66	CPS1
ATOM	583	CD	GLN	75	62.300	58.137	-9.295	1.00	32.50	CPS1
ATOM	584	OE1	GLN	75	61.673	57.207	-9.816	1.00	34.26	CPS1
ATOM	585	NE2	GLN	75	63.571	58.396	-9.584	1.00	30.64	CPS1
ATOM	586	C	GLN	75	64.052	58.543	-5.294	1.00	30.56	CPS1
ATOM	587	O	GLN	75	65.205	58.768	-5.681	1.00	29.97	CPS1
ATOM	588	N	ASP	76	63.697	58.605	-4.011	1.00	30.64	CPS1
ATOM	589	CA	ASP	76	64.669	58.943	-2.972	1.00	29.57	CPS1
ATOM	590	CB	ASP	76	63.975	59.494	-1.718	1.00	30.95	CPS1
ATOM	591	CG	ASP	76	63.293	60.824	-1.955	1.00	32.86	CPS1
ATOM	592	OD1	ASP	76	63.804	61.614	-2.771	1.00	33.98	CPS1
ATOM	593	OD2	ASP	76	62.254	61.083	-1.313	1.00	32.57	CPS1
ATOM	594	C	ASP	76	65.472	57.720	-2.546	1.00	28.65	CPS1
ATOM	595	O	ASP	76	66.430	57.835	-1.788	1.00	28.90	CPS1
ATOM	596	N	ILE	77	65.085	56.551	-3.038	1.00	27.41	CPS1
ATOM	597	CA	ILE	77	65.752	55.318	-2.644	1.00	26.26	CPS1
ATOM	598	CB	ILE	77	64.750	54.372	-1.947	1.00	25.85	CPS1
ATOM	599	CG2	ILE	77	65.494	53.213	-1.295	1.00	26.27	CPS1
ATOM	600	CG1	ILE	77	63.927	55.145	-0.912	1.00	25.55	CPS1
ATOM	601	CD1	ILE	77	62.613	54.455	-0.547	1.00	25.71	CPS1
ATOM	602	C	ILE	77	66.323	54.562	-3.830	1.00	26.41	CPS1
ATOM	603	O	ILE	77	65.633	54.355	-4.819	1.00	28.03	CPS1
ATOM	604	N	GLU	78	67.573	54.134	-3.726	1.00	26.24	CPS1
ATOM	605	CA	GLU	78	68.179	53.359	-4.800	1.00	26.41	CPS1
ATOM	606	CB	GLU	78	69.198	54.197	-5.586	1.00	27.49	CPS1
ATOM	607	CG	GLU	78	69.942	53.392	-6.661	1.00	31.00	CPS1
ATOM	608	CD	GLU	78	70.711	54.265	-7.657	1.00	34.35	CPS1
ATOM	609	OE1	GLU	78	70.059	54.887	-8.526	1.00	35.58	CPS1
ATOM	610	OE2	GLU	78	71.959	54.328	-7.568	1.00	34.83	CPS1
ATOM	611	C	GLU	78	68.856	52.116	-4.235	1.00	26.51	CPS1
ATOM	612	O	GLU	78	69.581	52.183	-3.244	1.00	26.47	CPS1
ATOM	613	N	ILE	79	68.595	50.976	-4.863	1.00	26.08	CPS1
ATOM	614	CA	ILE	79	69.205	49.731	-4.445	1.00	25.84	CPS1
ATOM	615	CB	ILE	79	68.192	48.545	-4.459	1.00	25.79	CPS1
ATOM	616	CG2	ILE	79	68.942	47.221	-4.467	1.00	25.99	CPS1
ATOM	617	CG1	ILE	79	67.282	48.595	-3.224	1.00	28.30	CPS1
ATOM	618	CD1	ILE	79	66.246	49.685	-3.247	1.00	25.92	CPS1
ATOM	619	C	ILE	79	70.329	49.419	-5.420	1.00	26.11	CPS1
ATOM	620	O	ILE	79	70.186	49.598	-6.633	1.00	24.92	CPS1
ATOM	621	N	ARG	80	71.455	48.974	-4.876	1.00	26.85	CPS1
ATOM	622	CA	ARG	80	72.604	48.582	-5.675	1.00	26.89	CPS1
ATOM	623	CB	ARG	80	73.708	49.616	-5.587	1.00	29.63	CPS1
ATOM	624	CG	ARG	80	73.353	50.965	-6.123	1.00	31.02	CPS1
ATOM	625	CD	ARG	80	74.524	51.844	-5.838	1.00	35.09	CPS1
ATOM	626	NE	ARG	80	74.282	53.237	-6.147	1.00	35.47	CPS1

FIG. 1A-11

ATOM	627	CZ	ARG	80	75.084	54.205	-5.736	1.00	33.96	CPS1
ATOM	628	NH1	ARG	80	76.149	53.896	-5.009	1.00	32.40	CPS1
ATOM	629	NH2	ARG	80	74.824	55.460	-6.053	1.00	34.37	CPS1
ATOM	630	C	ARG	80	73.130	47.294	-5.090	1.00	27.91	CPS1
ATOM	631	O	ARG	80	72.704	46.877	-4.017	1.00	26.72	CPS1
ATOM	632	N	LYS	81	74.061	46.662	-5.794	1.00	28.40	CPS1
ATOM	633	CA	LYS	81	74.671	45.436	-5.301	1.00	29.29	CPS1
ATOM	634	CB	LYS	81	74.395	44.275	-6.260	1.00	31.32	CPS1
ATOM	635	CG	LYS	81	72.962	43.773	-6.177	1.00	34.37	CPS1
ATOM	636	CD	LYS	81	72.745	42.490	-6.965	1.00	38.80	CPS1
ATOM	637	CE	LYS	81	71.388	41.887	-6.623	1.00	41.39	CPS1
ATOM	638	NZ	LYS	81	71.175	40.558	-7.270	1.00	45.04	CPS1
ATOM	639	C	LYS	81	76.159	45.688	-5.173	1.00	29.85	CPS1
ATOM	640	O	LYS	81	76.754	46.332	-6.039	1.00	29.65	CPS1
ATOM	641	N	ASP	82	76.768	45.225	-4.088	1.00	28.96	CPS1
ATOM	642	CA	ASP	82	78.194	45.443	-3.952	1.00	29.85	CPS1
ATOM	643	CB	ASP	82	78.642	45.423	-2.480	1.00	29.47	CPS1
ATOM	644	CG	ASP	82	78.413	44.095	-1.796	1.00	28.92	CPS1
ATOM	645	OD1	ASP	82	78.331	43.051	-2.471	1.00	29.25	CPS1
ATOM	646	OD2	ASP	82	78.346	44.105	-0.552	1.00	30.21	CPS1
ATOM	647	C	ASP	82	78.918	44.388	-4.773	1.00	30.66	CPS1
ATOM	648	O	ASP	82	78.281	43.626	-5.496	1.00	29.93	CPS1
ATOM	649	N	GLN	83	80.239	44.342	-4.667	1.00	32.99	CPS1
ATOM	650	CA	GLN	83	81.023	43.394	-5.450	1.00	34.77	CPS1
ATOM	651	CB	GLN	83	82.512	43.700	-5.287	1.00	37.08	CPS1
ATOM	652	CG	GLN	83	82.860	45.145	-5.635	1.00	38.94	CPS1
ATOM	653	CD	GLN	83	84.352	45.399	-5.653	1.00	40.99	CPS1
ATOM	654	OE1	GLN	83	85.032	45.115	-6.643	1.00	42.58	CPS1
ATOM	655	NE2	GLN	83	84.874	45.925	-4.549	1.00	41.73	CPS1
ATOM	656	C	GLN	83	80.746	41.924	-5.151	1.00	35.50	CPS1
ATOM	657	O	GLN	83	81.123	41.056	-5.930	1.00	35.54	CPS1
ATOM	658	N	ASN	84	80.094	41.640	-4.027	1.00	36.07	CPS1
ATOM	659	CA	ASN	84	79.757	40.258	-3.684	1.00	35.57	CPS1
ATOM	660	CB	ASN	84	79.863	40.014	-2.178	1.00	37.57	CPS1
ATOM	661	CG	ASN	84	81.284	39.960	-1.700	1.00	39.82	CPS1
ATOM	662	OD1	ASN	84	82.116	39.250	-2.270	1.00	41.25	CPS1
ATOM	663	ND2	ASN	84	81.577	40.702	-0.639	1.00	40.86	CPS1
ATOM	664	C	ASN	84	78.335	39.937	-4.113	1.00	34.27	CPS1
ATOM	665	O	ASN	84	77.856	38.824	-3.899	1.00	34.98	CPS1
ATOM	666	N	GLY	85	77.659	40.914	-4.706	1.00	31.13	CPS1
ATOM	667	CA	GLY	85	76.289	40.703	-5.137	1.00	29.50	CPS1
ATOM	668	C	GLY	85	75.274	41.002	-4.040	1.00	27.83	CPS1
ATOM	669	O	GLY	85	74.089	40.743	-4.209	1.00	27.44	CPS1
ATOM	670	N	LYS	86	75.737	41.548	-2.919	1.00	26.25	CPS1
ATOM	671	CA	LYS	86	74.858	41.888	-1.797	1.00	25.96	CPS1
ATOM	672	CB	LYS	86	75.664	41.946	-0.500	1.00	26.50	CPS1
ATOM	673	CG	LYS	86	74.905	42.542	0.680	1.00	26.15	CPS1
ATOM	674	CD	LYS	86	73.833	41.595	1.234	1.00	24.85	CPS1
ATOM	675	CE	LYS	86	73.002	42.312	2.322	1.00	24.53	CPS1
ATOM	676	NZ	LYS	86	72.000	41.403	2.973	1.00	23.95	CPS1
ATOM	677	C	LYS	86	74.164	43.232	-2.002	1.00	24.92	CPS1
ATOM	678	O	LYS	86	74.812	44.253	-2.223	1.00	25.51	CPS1
ATOM	679	N	PRO	87	72.830	43.256	-1.938	1.00	24.79	CPS1
ATOM	680	CD	PRO	87	71.858	42.148	-1.905	1.00	26.28	CPS1
ATOM	681	CA	PRO	87	72.157	44.538	-2.123	1.00	23.90	CPS1
ATOM	682	CB	PRO	87	70.702	44.136	-2.356	1.00	25.37	CPS1
ATOM	683	CG	PRO	87	70.571	42.868	-1.581	1.00	26.57	CPS1

FIG. 1A-12

ATOM	684	C	PRO	87	72.300	45.486	-0.933	1.00	24.14	CPS1
ATOM	685	O	PRO	87	72.355	45.061	0.222	1.00	23.36	CPS1
ATOM	686	N	TYR	88	72.383	46.775	-1.223	1.00	23.09	CPS1
ATOM	687	CA	TYR	88	72.456	47.775	-0.170	1.00	22.80	CPS1
ATOM	688	CB	TYR	88	73.903	48.132	0.169	1.00	23.97	CPS1
ATOM	689	CG	TYR	88	74.662	48.796	-0.948	1.00	23.15	CPS1
ATOM	690	CD1	TYR	88	74.617	50.176	-1.121	1.00	23.81	CPS1
ATOM	691	CE1	TYR	88	75.334	50.803	-2.148	1.00	24.04	CPS1
ATOM	692	CD2	TYR	88	75.438	48.042	-1.823	1.00	23.00	CPS1
ATOM	693	CE2	TYR	88	76.163	48.653	-2.853	1.00	23.00	CPS1
ATOM	694	CZ	TYR	88	76.106	50.031	-3.007	1.00	24.59	CPS1
ATOM	695	OH	TYR	88	76.807	50.635	-4.029	1.00	23.69	CPS1
ATOM	696	C	TYR	88	71.697	48.978	-0.676	1.00	24.07	CPS1
ATOM	697	O	TYR	88	71.492	49.131	-1.882	1.00	24.63	CPS1
ATOM	698	N	ILE	89	71.265	49.821	0.247	1.00	23.90	CPS1
ATOM	699	CA	ILE	89	70.486	50.992	-0.096	1.00	24.96	CPS1
ATOM	700	CB	ILE	89	69.183	51.038	0.763	1.00	25.43	CPS1
ATOM	701	CG2	ILE	89	68.580	52.445	0.773	1.00	23.76	CPS1
ATOM	702	CG1	ILE	89	68.179	50.007	0.237	1.00	25.76	CPS1
ATOM	703	CD1	ILE	89	66.920	49.857	1.102	1.00	25.48	CPS1
ATOM	704	C	ILE	89	71.230	52.304	0.086	1.00	26.98	CPS1
ATOM	705	O	ILE	89	72.018	52.470	1.020	1.00	27.02	CPS1
ATOM	706	N	ILE	90	70.984	53.227	-0.840	1.00	28.88	CPS1
ATOM	707	CA	ILE	90	71.543	54.567	-0.750	1.00	31.89	CPS1
ATOM	708	CB	ILE	90	72.383	54.968	-1.983	1.00	34.52	CPS1
ATOM	709	CG2	ILE	90	72.685	56.465	-1.930	1.00	35.39	CPS1
ATOM	710	CG1	ILE	90	73.692	54.176	-2.020	1.00	34.95	CPS1
ATOM	711	CD1	ILE	90	74.585	54.381	-0.812	1.00	36.25	CPS1
ATOM	712	C	ILE	90	70.299	55.433	-0.715	1.00	32.42	CPS1
ATOM	713	O	ILE	90	69.450	55.342	-1.599	1.00	32.97	CPS1
ATOM	714	N	CYS	91	70.165	56.246	0.320	1.00	32.73	CPS1
ATOM	715	CA	CYS	91	69.002	57.106	0.433	1.00	34.96	CPS1
ATOM	716	CB	CYS	91	68.008	56.543	1.463	1.00	32.49	CPS1
ATOM	717	SG	CYS	91	66.523	57.557	1.657	1.00	29.59	CPS1
ATOM	718	C	CYS	91	69.452	58.494	0.848	1.00	38.10	CPS1
ATOM	719	O	CYS	91	70.079	58.666	1.893	1.00	40.46	CPS1
ATOM	720	N	THR	92	69.124	59.476	0.014	1.00	42.14	CPS1
ATOM	721	CA	THR	92	69.489	60.870	0.246	1.00	45.56	CPS1
ATOM	722	CB	THR	92	68.964	61.772	-0.898	1.00	46.93	CPS1
ATOM	723	OG1	THR	92	67.552	61.562	-1.069	1.00	48.39	CPS1
ATOM	724	CG2	THR	92	69.686	61.454	-2.205	1.00	47.93	CPS1
ATOM	725	C	THR	92	69.001	61.457	1.571	1.00	46.35	CPS1
ATOM	726	O	THR	92	69.345	62.592	1.901	1.00	47.51	CPS1
ATOM	727	N	LYS	93	68.211	60.703	2.332	1.00	46.09	CPS1
ATOM	728	CA	LYS	93	67.714	61.218	3.602	1.00	46.14	CPS1
ATOM	729	CB	LYS	93	66.214	60.944	3.725	1.00	46.87	CPS1
ATOM	730	CG	LYS	93	65.395	61.870	2.837	1.00	48.42	CPS1
ATOM	731	CD	LYS	93	63.903	61.704	3.034	1.00	49.49	CPS1
ATOM	732	CE	LYS	93	63.148	62.908	2.482	1.00	50.63	CPS1
ATOM	733	NZ	LYS	93	63.471	63.177	1.054	1.00	52.22	CPS1
ATOM	734	C	LYS	93	68.452	60.733	4.844	1.00	45.50	CPS1
ATOM	735	O	LYS	93	68.167	61.182	5.954	1.00	45.52	CPS1
ATOM	736	N	LEU	94	69.408	59.829	4.657	1.00	44.83	CPS1
ATOM	737	CA	LEU	94	70.200	59.313	5.770	1.00	44.48	CPS1
ATOM	738	CB	LEU	94	69.376	58.330	6.611	1.00	44.44	CPS1
ATOM	739	CG	LEU	94	68.488	57.283	5.928	1.00	44.15	CPS1
ATOM	740	CD1	LEU	94	69.258	56.498	4.886	1.00	42.30	CPS1

FIG. 1A-13

ATOM	741	CD2	LEU	94	67.934	56.361	6.997	1.00	43.28	CPS1
ATOM	742	C	LEU	94	71.486	58.641	5.307	1.00	44.30	CPS1
ATOM	743	O	LEU	94	71.692	58.432	4.111	1.00	44.84	CPS1
ATOM	744	N	SER	95	72.353	58.308	6.257	1.00	43.56	CPS1
ATOM	745	CA	SER	95	73.612	57.655	5.934	1.00	44.17	CPS1
ATOM	746	CB	SER	95	74.583	57.748	7.107	1.00	44.85	CPS1
ATOM	747	OG	SER	95	75.803	57.098	6.784	1.00	47.82	CPS1
ATOM	748	C	SER	95	73.408	56.184	5.577	1.00	43.59	CPS1
ATOM	749	O	SER	95	72.676	55.462	6.258	1.00	43.06	CPS1
ATOM	750	N	PRO	96	74.065	55.720	4.503	1.00	42.46	CPS1
ATOM	751	CD	PRO	96	75.025	56.444	3.650	1.00	42.90	CPS1
ATOM	752	CA	PRO	96	73.939	54.325	4.079	1.00	41.30	CPS1
ATOM	753	CB	PRO	96	74.757	54.286	2.788	1.00	42.08	CPS1
ATOM	754	CG	PRO	96	75.821	55.316	3.045	1.00	42.41	CPS1
ATOM	755	C	PRO	96	74.473	53.379	5.153	1.00	39.30	CPS1
ATOM	756	O	PRO	96	74.098	52.210	5.206	1.00	38.17	CPS1
ATOM	757	N	ALA	97	75.348	53.901	6.008	1.00	37.86	CPS1
ATOM	758	CA	ALA	97	75.929	53.117	7.095	1.00	36.05	CPS1
ATOM	759	CB	ALA	97	76.982	53.940	7.819	1.00	37.73	CPS1
ATOM	760	C	ALA	97	74.857	52.681	8.090	1.00	35.10	CPS1
ATOM	761	O	ALA	97	74.992	51.662	8.770	1.00	35.38	CPS1
ATOM	762	N	ALA	98	73.789	53.460	8.173	1.00	33.38	CPS1
ATOM	763	CA	ALA	98	72.717	53.160	9.107	1.00	31.76	CPS1
ATOM	764	CB	ALA	98	72.057	54.454	9.546	1.00	33.83	CPS1
ATOM	765	C	ALA	98	71.657	52.220	8.537	1.00	30.24	CPS1
ATOM	766	O	ALA	98	70.734	51.849	9.255	1.00	31.14	CPS1
ATOM	767	N	VAL	99	71.796	51.831	7.269	1.00	26.77	CPS1
ATOM	768	CA	VAL	99	70.803	50.980	6.607	1.00	25.25	CPS1
ATOM	769	CB	VAL	99	70.258	51.695	5.331	1.00	24.54	CPS1
ATOM	770	CG1	VAL	99	69.091	50.920	4.731	1.00	24.61	CPS1
ATOM	771	CG2	VAL	99	69.829	53.107	5.676	1.00	26.14	CPS1
ATOM	772	C	VAL	99	71.272	49.576	6.207	1.00	23.74	CPS1
ATOM	773	O	VAL	99	72.390	49.393	5.720	1.00	23.55	CPS1
ATOM	774	N	HIS	100	70.395	48.595	6.422	1.00	22.48	CPS1
ATOM	775	CA	HIS	100	70.640	47.195	6.075	1.00	21.75	CPS1
ATOM	776	CB	HIS	100	70.873	46.360	7.334	1.00	23.99	CPS1
ATOM	777	CG	HIS	100	72.020	46.846	8.160	1.00	27.42	CPS1
ATOM	778	CD2	HIS	100	72.060	47.696	9.212	1.00	28.79	CPS1
ATOM	779	ND1	HIS	100	73.329	46.542	7.859	1.00	28.14	CPS1
ATOM	780	CE1	HIS	100	74.128	47.190	8.689	1.00	30.71	CPS1
ATOM	781	NE2	HIS	100	73.383	47.898	9.519	1.00	30.58	CPS1
ATOM	782	C	HIS	100	69.394	46.686	5.357	1.00	20.99	CPS1
ATOM	783	O	HIS	100	68.270	47.007	5.752	1.00	20.00	CPS1
ATOM	784	N	VAL	101	69.593	45.893	4.312	1.00	20.41	CPS1
ATOM	785	CA	VAL	101	68.473	45.357	3.551	1.00	20.21	CPS1
ATOM	786	CB	VAL	101	68.181	46.244	2.290	1.00	20.23	CPS1
ATOM	787	CG1	VAL	101	69.391	46.245	1.344	1.00	22.43	CPS1
ATOM	788	CG2	VAL	101	66.958	45.723	1.553	1.00	21.20	CPS1
ATOM	789	C	VAL	101	68.761	43.939	3.084	1.00	20.38	CPS1
ATOM	790	O	VAL	101	69.920	43.527	2.986	1.00	19.26	CPS1
ATOM	791	N	SER	102	67.702	43.167	2.835	1.00	19.19	CPS1
ATOM	792	CA	SER	102	67.867	41.833	2.280	1.00	19.46	CPS1
ATOM	793	CB	SER	102	67.884	40.742	3.345	1.00	18.79	CPS1
ATOM	794	OG	SER	102	68.068	39.478	2.720	1.00	18.64	CPS1
ATOM	795	C	SER	102	66.677	41.638	1.358	1.00	20.37	CPS1
ATOM	796	O	SER	102	65.581	42.095	1.658	1.00	20.10	CPS1
ATOM	797	N	ILE	103	66.902	40.964	0.236	1.00	19.92	CPS1

FIG. 1A-14

ATOM	798	CA	ILE	103	65.847	40.737	-0.744	1.00	19.71	CPS1
ATOM	799	CB	ILE	103	66.122	41.550	-2.033	1.00	19.02	CPS1
ATOM	800	CG2	ILE	103	64.988	41.337	-3.054	1.00	19.50	CPS1
ATOM	801	CG1	ILE	103	66.234	43.031	-1.682	1.00	18.90	CPS1
ATOM	802	CD1	ILE	103	66.767	43.904	-2.828	1.00	19.01	CPS1
ATOM	803	C	ILE	103	65.804	39.265	-1.090	1.00	20.30	CPS1
ATOM	804	O	ILE	103	66.847	38.620	-1.164	1.00	20.97	CPS1
ATOM	805	N	THR	104	64.603	38.729	-1.287	1.00	20.48	CPS1
ATOM	806	CA	THR	104	64.468	37.316	-1.623	1.00	20.34	CPS1
ATOM	807	CB	THR	104	64.172	36.462	-0.350	1.00	21.86	CPS1
ATOM	808	OG1	THR	104	64.222	35.065	-0.671	1.00	21.77	CPS1
ATOM	809	CG2	THR	104	62.804	36.795	0.213	1.00	20.65	CPS1
ATOM	810	C	THR	104	63.346	37.139	-2.642	1.00	21.68	CPS1
ATOM	811	O	THR	104	62.501	38.018	-2.813	1.00	20.50	CPS1
ATOM	812	N	HIS	105	63.345	36.003	-3.325	1.00	22.11	CPS1
ATOM	813	CA	HIS	105	62.323	35.728	-4.331	1.00	24.82	CPS1
ATOM	814	CB	HIS	105	62.884	35.948	-5.747	1.00	27.53	CPS1
ATOM	815	CG	HIS	105	63.383	37.335	-6.020	1.00	32.22	CPS1
ATOM	816	CD2	HIS	105	64.585	37.915	-5.782	1.00	34.13	CPS1
ATOM	817	ND1	HIS	105	62.615	38.292	-6.648	1.00	36.59	CPS1
ATOM	818	CE1	HIS	105	63.322	39.402	-6.786	1.00	35.80	CPS1
ATOM	819	NE2	HIS	105	64.521	39.199	-6.271	1.00	35.22	CPS1
ATOM	820	C	HIS	105	61.863	34.268	-4.280	1.00	24.66	CPS1
ATOM	821	O	HIS	105	62.570	33.400	-3.766	1.00	23.89	CPS1
ATOM	822	N	THR	106	60.667	34.027	-4.811	1.00	24.24	CPS1
ATOM	823	CA	THR	106	60.127	32.677	-5.003	1.00	24.46	CPS1
ATOM	824	CB	THR	106	59.008	32.271	-4.019	1.00	25.81	CPS1
ATOM	825	OG1	THR	106	57.840	33.073	-4.253	1.00	25.01	CPS1
ATOM	826	CG2	THR	106	59.483	32.419	-2.570	1.00	24.51	CPS1
ATOM	827	C	THR	106	59.500	32.820	-6.388	1.00	25.67	CPS1
ATOM	828	O	THR	106	59.496	33.915	-6.953	1.00	25.60	CPS1
ATOM	829	N	ALA	107	58.962	31.740	-6.939	1.00	25.39	CPS1
ATOM	830	CA	ALA	107	58.355	31.824	-8.262	1.00	25.43	CPS1
ATOM	831	CB	ALA	107	57.743	30.463	-8.637	1.00	25.15	CPS1
ATOM	832	C	ALA	107	57.288	32.918	-8.363	1.00	25.95	CPS1
ATOM	833	O	ALA	107	57.233	33.660	-9.353	1.00	25.81	CPS1
ATOM	834	N	GLU	108	56.452	33.035	-7.335	1.00	24.82	CPS1
ATOM	835	CA	GLU	108	55.356	34.007	-7.367	1.00	25.17	CPS1
ATOM	836	CB	GLU	108	54.043	33.295	-7.008	1.00	27.79	CPS1
ATOM	837	CG	GLU	108	53.688	32.198	-8.005	1.00	34.77	CPS1
ATOM	838	CD	GLU	108	52.404	31.450	-7.675	1.00	39.77	CPS1
ATOM	839	OE1	GLU	108	52.146	30.431	-8.355	1.00	43.18	CPS1
ATOM	840	OE2	GLU	108	51.652	31.864	-6.758	1.00	42.25	CPS1
ATOM	841	C	GLU	108	55.486	35.267	-6.507	1.00	24.23	CPS1
ATOM	842	O	GLU	108	54.654	36.178	-6.615	1.00	22.93	CPS1
ATOM	843	N	TYR	109	56.518	35.330	-5.669	1.00	21.86	CPS1
ATOM	844	CA	TYR	109	56.678	36.480	-4.788	1.00	21.64	CPS1
ATOM	845	CB	TYR	109	56.320	36.077	-3.352	1.00	22.31	CPS1
ATOM	846	CG	TYR	109	54.889	35.632	-3.180	1.00	23.87	CPS1
ATOM	847	CD1	TYR	109	53.868	36.562	-2.999	1.00	23.05	CPS1
ATOM	848	CE1	TYR	109	52.546	36.164	-2.894	1.00	24.80	CPS1
ATOM	849	CD2	TYR	109	54.550	34.283	-3.253	1.00	24.86	CPS1
ATOM	850	CE2	TYR	109	53.226	33.872	-3.154	1.00	27.10	CPS1
ATOM	851	CZ	TYR	109	52.233	34.818	-2.977	1.00	24.92	CPS1
ATOM	852	OH	TYR	109	50.924	34.420	-2.916	1.00	25.87	CPS1
ATOM	853	C	TYR	109	58.066	37.100	-4.741	1.00	21.01	CPS1
ATOM	854	O	TYR	109	59.063	36.476	-5.091	1.00	21.94	CPS1

FIG. 1A-15

ATOM	855	N	ALA	110	58.097	38.347	-4.292	1.00 20.81	CPS1
ATOM	856	CA	ALA	110	59.344	39.074	-4.057	1.00 20.89	CPS1
ATOM	857	CB	ALA	110	59.483	40.256	-5.013	1.00 21.11	CPS1
ATOM	858	C	ALA	110	59.155	39.574	-2.617	1.00 19.96	CPS1
ATOM	859	O	ALA	110	58.043	39.941	-2.238	1.00 21.37	CPS1
ATOM	860	N	ALA	111	60.209	39.576	-1.805	1.00 18.57	CPS1
ATOM	861	CA	ALA	111	60.074	40.062	-0.435	1.00 17.40	CPS1
ATOM	862	CB	ALA	111	59.780	38.896	0.509	1.00 16.67	CPS1
ATOM	863	C	ALA	111	61.362	40.756	-0.023	1.00 17.97	CPS1
ATOM	864	O	ALA	111	62.411	40.476	-0.580	1.00 17.28	CPS1
ATOM	865	N	ALA	112	61.275	41.676	0.931	1.00 16.46	CPS1
ATOM	866	CA	ALA	112	62.458	42.374	1.394	1.00 17.56	CPS1
ATOM	867	CB	ALA	112	62.786	43.553	0.444	1.00 17.14	CPS1
ATOM	868	C	ALA	112	62.263	42.880	2.809	1.00 16.81	CPS1
ATOM	869	O	ALA	112	61.143	43.042	3.270	1.00 17.67	CPS1
ATOM	870	N	GLN	113	63.361	43.106	3.514	1.00 17.77	CPS1
ATOM	871	CA	GLN	113	63.267	43.639	4.863	1.00 17.30	CPS1
ATOM	872	CB	GLN	113	63.469	42.554	5.929	1.00 18.78	CPS1
ATOM	873	CG	GLN	113	64.842	41.925	5.912	1.00 22.22	CPS1
ATOM	874	CD	GLN	113	65.029	40.878	6.990	1.00 26.02	CPS1
ATOM	875	OE1	GLN	113	66.130	40.366	7.182	1.00 29.00	CPS1
ATOM	876	NE2	GLN	113	63.950	40.541	7.688	1.00 28.62	CPS1
ATOM	877	C	GLN	113	64.370	44.658	4.985	1.00 18.39	CPS1
ATOM	878	O	GLN	113	65.410	44.550	4.338	1.00 19.07	CPS1
ATOM	879	N	VAL	114	64.142	45.639	5.836	1.00 18.02	CPS1
ATOM	880	CA	VAL	114	65.128	46.675	6.042	1.00 17.24	CPS1
ATOM	881	CB	VAL	114	64.702	47.987	5.317	1.00 17.08	CPS1
ATOM	882	CG1	VAL	114	65.511	49.194	5.863	1.00 16.82	CPS1
ATOM	883	CG2	VAL	114	64.897	47.837	3.810	1.00 15.69	CPS1
ATOM	884	C	VAL	114	65.223	46.962	7.526	1.00 18.35	CPS1
ATOM	885	O	VAL	114	64.228	46.862	8.260	1.00 17.93	CPS1
ATOM	886	N	VAL	115	66.429	47.280	7.973	1.00 19.07	CPS1
ATOM	887	CA	VAL	115	66.622	47.702	9.351	1.00 20.05	CPS1
ATOM	888	CB	VAL	115	67.435	46.698	10.193	1.00 21.79	CPS1
ATOM	889	CG1	VAL	115	67.695	47.297	11.582	1.00 24.02	CPS1
ATOM	890	CG2	VAL	115	66.680	45.387	10.322	1.00 21.49	CPS1
ATOM	891	C	VAL	115	67.411	49.003	9.266	1.00 20.53	CPS1
ATOM	892	O	VAL	115	68.416	49.077	8.552	1.00 19.46	CPS1
ATOM	893	N	ILE	116	66.921	50.038	9.943	1.00 22.12	CPS1
ATOM	894	CA	ILE	116	67.620	51.321	9.987	1.00 22.75	CPS1
ATOM	895	CB	ILE	116	66.694	52.492	9.629	1.00 22.88	CPS1
ATOM	896	CG2	ILE	116	67.430	53.825	9.850	1.00 23.51	CPS1
ATOM	897	CG1	ILE	116	66.232	52.353	8.172	1.00 22.44	CPS1
ATOM	898	CD1	ILE	116	65.208	53.382	7.742	1.00 20.81	CPS1
ATOM	899	C	ILE	116	68.090	51.495	11.430	1.00 25.25	CPS1
ATOM	900	O	ILE	116	67.312	51.296	12.363	1.00 22.08	CPS1
ATOM	901	N	GLU	117	69.362	51.845	11.610	1.00 28.24	CPS1
ATOM	902	CA	GLU	117	69.923	52.041	12.944	1.00 33.38	CPS1
ATOM	903	CB	GLU	117	71.297	51.384	13.074	1.00 34.32	CPS1
ATOM	904	CG	GLU	117	71.376	49.888	12.878	1.00 36.79	CPS1
ATOM	905	CD	GLU	117	72.808	49.388	13.006	1.00 38.57	CPS1
ATOM	906	OE1	GLU	117	73.266	49.163	14.144	1.00 40.54	CPS1
ATOM	907	OE2	GLU	117	73.489	49.243	11.971	1.00 40.35	CPS1
ATOM	908	C	GLU	117	70.119	53.524	13.216	1.00 36.51	CPS1
ATOM	909	O	GLU	117	70.269	54.317	12.289	1.00 36.14	CPS1
ATOM	910	N	ARG	118	70.120	53.890	14.493	1.00 40.58	CPS1
ATOM	911	CA	ARG	118	70.358	55.275	14.884	1.00 45.79	CPS1

FIG. 1A-16

ATOM	912	CB	ARG	118	69.712	55.600	16.235	1.00 46.59	CPS1
ATOM	913	CG	ARG	118	68.229	55.336	16.356	1.00 49.65	CPS1
ATOM	914	CD	ARG	118	67.792	55.527	17.809	1.00 52.26	CPS1
ATOM	915	NE	ARG	118	66.418	55.092	18.046	1.00 54.79	CPS1
ATOM	916	CZ	ARG	118	65.337	55.786	17.702	1.00 55.39	CPS1
ATOM	917	NH1	ARG	118	64.131	55.299	17.956	1.00 56.47	CPS1
ATOM	918	NH2	ARG	118	65.458	56.972	17.120	1.00 56.32	CPS1
ATOM	919	C	ARG	118	71.868	55.331	15.069	1.00 48.09	CPS1
ATOM	920	O	ARG	118	72.435	54.481	15.755	1.00 49.38	CPS1
ATOM	921	N	LEU	119	72.529	56.308	14.462	1.00 50.93	CPS1
ATOM	922	CA	LEU	119	73.973	56.418	14.631	1.00 53.26	CPS1
ATOM	923	CB	LEU	119	74.651	56.655	13.277	1.00 53.81	CPS1
ATOM	924	CG	LEU	119	74.474	55.541	12.239	1.00 54.33	CPS1
ATOM	925	CD1	LEU	119	75.203	55.906	10.953	1.00 54.92	CPS1
ATOM	926	CD2	LEU	119	75.006	54.234	12.801	1.00 54.83	CPS1
ATOM	927	C	LEU	119	74.286	57.568	15.591	1.00 54.40	CPS1
ATOM	928	OT1	LEU	119	74.613	57.278	16.765	1.00 55.09	CPS1
ATOM	929	OT2	LEU	119	74.177	58.740	15.166	1.00 55.10	CPS1
ATOM	930	C	GLY	0	77.740	47.623	17.259	1.00 45.52	CPS2
ATOM	931	O	GLY	0	78.476	48.184	16.444	1.00 47.54	CPS2
ATOM	932	N	GLY	0	79.569	47.872	18.959	1.00 47.48	CPS2
ATOM	933	CA	GLY	0	78.237	47.280	18.650	1.00 46.63	CPS2
ATOM	934	N	GLY	1	76.484	47.284	16.983	1.00 43.42	CPS2
ATOM	935	CA	GLY	1	75.916	47.570	15.679	1.00 38.90	CPS2
ATOM	936	C	GLY	1	75.631	46.308	14.888	1.00 35.36	CPS2
ATOM	937	O	GLY	1	76.138	45.233	15.198	1.00 35.52	CPS2
ATOM	938	N	ILE	2	74.818	46.451	13.853	1.00 32.81	CPS2
ATOM	939	CA	ILE	2	74.444	45.331	12.997	1.00 30.92	CPS2
ATOM	940	CB	ILE	2	73.034	45.554	12.419	1.00 30.17	CPS2
ATOM	941	CG2	ILE	2	72.715	44.495	11.369	1.00 28.15	CPS2
ATOM	942	CG1	ILE	2	72.019	45.547	13.564	1.00 30.04	CPS2
ATOM	943	CD1	ILE	2	70.624	45.977	13.162	1.00 29.29	CPS2
ATOM	944	C	ILE	2	75.427	45.143	11.851	1.00 30.22	CPS2
ATOM	945	O	ILE	2	75.785	46.098	11.157	1.00 29.17	CPS2
ATOM	946	N	TYR	3	75.866	43.906	11.657	1.00 29.82	CPS2
ATOM	947	CA	TYR	3	76.797	43.596	10.577	1.00 29.72	CPS2
ATOM	948	CB	TYR	3	77.594	42.334	10.900	1.00 32.80	CPS2
ATOM	949	CG	TYR	3	78.536	41.959	9.782	1.00 37.46	CPS2
ATOM	950	CD1	TYR	3	79.553	42.827	9.394	1.00 39.59	CPS2
ATOM	951	CE1	TYR	3	80.382	42.538	8.314	1.00 42.43	CPS2
ATOM	952	CD2	TYR	3	78.370	40.775	9.064	1.00 39.81	CPS2
ATOM	953	CE2	TYR	3	79.196	40.470	7.974	1.00 42.42	CPS2
ATOM	954	CZ	TYR	3	80.201	41.364	7.607	1.00 44.04	CPS2
ATOM	955	OH	TYR	3	81.024	41.099	6.531	1.00 46.34	CPS2
ATOM	956	C	TYR	3	76.032	43.379	9.275	1.00 28.30	CPS2
ATOM	957	O	TYR	3	76.420	43.872	8.211	1.00 28.24	CPS2
ATOM	958	N	GLY	4	74.944	42.619	9.363	1.00 25.87	CPS2
ATOM	959	CA	GLY	4	74.141	42.355	8.182	1.00 22.75	CPS2
ATOM	960	C	GLY	4	72.849	41.652	8.547	1.00 21.62	CPS2
ATOM	961	O	GLY	4	72.724	41.085	9.639	1.00 21.41	CPS2
ATOM	962	N	ILE	5	71.877	41.703	7.640	1.00 20.89	CPS2
ATOM	963	CA	ILE	5	70.593	41.042	7.859	1.00 19.45	CPS2
ATOM	964	CB	ILE	5	69.453	42.057	8.118	1.00 18.65	CPS2
ATOM	965	CG2	ILE	5	69.846	43.011	9.259	1.00 19.69	CPS2
ATOM	966	CG1	ILE	5	69.129	42.843	6.842	1.00 19.64	CPS2
ATOM	967	CD1	ILE	5	67.947	43.809	7.020	1.00 20.64	CPS2
ATOM	968	C	ILE	5	70.272	40.216	6.618	1.00 18.82	CPS2

FIG. 1A-17

ATOM	969	O	ILE	5	70.778	40.498	5.524	1.00	18.88	CPS2
ATOM	970	N	GLY	6	69.456	39.184	6.794	1.00	19.17	CPS2
ATOM	971	CA	GLY	6	69.108	38.325	5.679	1.00	19.31	CPS2
ATOM	972	C	GLY	6	67.687	37.815	5.794	1.00	19.36	CPS2
ATOM	973	O	GLY	6	67.176	37.614	6.887	1.00	18.63	CPS2
ATOM	974	N	LEU	7	67.053	37.606	4.649	1.00	19.78	CPS2
ATOM	975	CA	LEU	7	65.680	37.141	4.617	1.00	19.08	CPS2
ATOM	976	CB	LEU	7	64.733	38.328	4.366	1.00	19.19	CPS2
ATOM	977	CG	LEU	7	63.238	38.018	4.161	1.00	18.29	CPS2
ATOM	978	CD1	LEU	7	62.658	37.539	5.491	1.00	18.90	CPS2
ATOM	979	CD2	LEU	7	62.472	39.269	3.651	1.00	17.44	CPS2
ATOM	980	C	LEU	7	65.552	36.139	3.487	1.00	18.38	CPS2
ATOM	981	O	LEU	7	66.113	36.338	2.417	1.00	19.54	CPS2
ATOM	982	N	ASP	8	64.845	35.042	3.724	1.00	18.51	CPS2
ATOM	983	CA	ASP	8	64.651	34.091	2.647	1.00	20.25	CPS2
ATOM	984	CB	ASP	8	65.727	32.998	2.657	1.00	21.81	CPS2
ATOM	985	CG	ASP	8	65.487	31.943	1.580	1.00	25.13	CPS2
ATOM	986	OD1	ASP	8	64.777	30.949	1.851	1.00	25.80	CPS2
ATOM	987	OD2	ASP	8	65.989	32.124	0.454	1.00	28.14	CPS2
ATOM	988	C	ASP	8	63.297	33.433	2.740	1.00	20.84	CPS2
ATOM	989	O	ASP	8	62.826	33.137	3.834	1.00	19.86	CPS2
ATOM	990	N	ILE	9	62.669	33.223	1.584	1.00	19.61	CPS2
ATOM	991	CA	ILE	9	61.391	32.520	1.533	1.00	20.19	CPS2
ATOM	992	CB	ILE	9	60.222	33.393	1.015	1.00	21.26	CPS2
ATOM	993	CG2	ILE	9	58.950	32.526	0.904	1.00	20.13	CPS2
ATOM	994	CG1	ILE	9	59.959	34.555	1.973	1.00	21.42	CPS2
ATOM	995	CD1	ILE	9	58.878	35.500	1.490	1.00	21.37	CPS2
ATOM	996	C	ILE	9	61.641	31.415	0.519	1.00	20.37	CPS2
ATOM	997	O	ILE	9	62.132	31.685	-0.572	1.00	20.53	CPS2
ATOM	998	N	THR	10	61.313	30.182	0.892	1.00	20.80	CPS2
ATOM	999	CA	THR	10	61.519	29.032	0.022	1.00	22.14	CPS2
ATOM	1000	CB	THR	10	62.584	28.076	0.630	1.00	23.02	CPS2
ATOM	1001	OG1	THR	10	63.837	28.770	0.746	1.00	25.04	CPS2
ATOM	1002	CG2	THR	10	62.785	26.859	-0.253	1.00	25.37	CPS2
ATOM	1003	C	THR	10	60.211	28.275	-0.184	1.00	21.99	CPS2
ATOM	1004	O	THR	10	59.471	28.038	0.761	1.00	21.01	CPS2
ATOM	1005	N	GLU	11	59.938	27.912	-1.435	1.00	23.31	CPS2
ATOM	1006	CA	GLU	11	58.723	27.177	-1.794	1.00	24.42	CPS2
ATOM	1007	CB	GLU	11	58.438	27.355	-3.296	1.00	26.52	CPS2
ATOM	1008	CG	GLU	11	57.052	26.900	-3.721	1.00	28.30	CPS2
ATOM	1009	CD	GLU	11	56.897	26.756	-5.231	1.00	32.57	CPS2
ATOM	1010	OE1	GLU	11	57.820	27.134	-5.991	1.00	32.18	CPS2
ATOM	1011	OE2	GLU	11	55.833	26.256	-5.654	1.00	33.69	CPS2
ATOM	1012	C	GLU	11	58.941	25.692	-1.480	1.00	23.56	CPS2
ATOM	1013	O	GLU	11	59.853	25.070	-2.026	1.00	22.90	CPS2
ATOM	1014	N	LEU	12	58.110	25.124	-0.612	1.00	23.91	CPS2
ATOM	1015	CA	LEU	12	58.260	23.715	-0.249	1.00	26.06	CPS2
ATOM	1016	CB	LEU	12	57.147	23.269	0.705	1.00	28.23	CPS2
ATOM	1017	CG	LEU	12	57.554	23.114	2.176	1.00	31.10	CPS2
ATOM	1018	CD1	LEU	12	58.046	24.448	2.710	1.00	30.63	CPS2
ATOM	1019	CD2	LEU	12	56.360	22.605	3.005	1.00	32.22	CPS2
ATOM	1020	C	LEU	12	58.271	22.795	-1.461	1.00	27.56	CPS2
ATOM	1021	O	LEU	12	59.054	21.846	-1.519	1.00	27.33	CPS2
ATOM	1022	N	ALA	13	57.401	23.077	-2.427	1.00	27.64	CPS2
ATOM	1023	CA	ALA	13	57.321	22.255	-3.628	1.00	28.06	CPS2
ATOM	1024	CB	ALA	13	56.163	22.714	-4.506	1.00	28.61	CPS2
ATOM	1025	C	ALA	13	58.622	22.279	-4.413	1.00	29.21	CPS2

FIG. 1A-18

ATOM	1026	O	ALA	13	58.982	21.281	-5.048	1.00	28.52	CPS2
ATOM	1027	N	ARG	14	59.335	23.404	-4.375	1.00	29.11	CPS2
ATOM	1028	CA	ARG	14	60.599	23.495	-5.098	1.00	30.50	CPS2
ATOM	1029	CB	ARG	14	61.065	24.951	-5.221	1.00	32.06	CPS2
ATOM	1030	CG	ARG	14	62.248	25.118	-6.171	1.00	34.92	CPS2
ATOM	1031	CD	ARG	14	62.528	26.576	-6.477	1.00	36.22	CPS2
ATOM	1032	NE	ARG	14	63.217	27.245	-5.381	1.00	38.47	CPS2
ATOM	1033	CZ	ARG	14	64.522	27.137	-5.142	1.00	39.99	CPS2
ATOM	1034	NH1	ARG	14	65.284	26.385	-5.926	1.00	39.47	CPS2
ATOM	1035	NH2	ARG	14	65.066	27.787	-4.119	1.00	39.80	CPS2
ATOM	1036	C	ARG	14	61.670	22.655	-4.411	1.00	30.84	CPS2
ATOM	1037	O	ARG	14	62.488	22.021	-5.077	1.00	31.28	CPS2
ATOM	1038	N	ILE	15	61.672	22.650	-3.078	1.00	31.04	CPS2
ATOM	1039	CA	ILE	15	62.637	21.845	-2.332	1.00	31.02	CPS2
ATOM	1040	CB	ILE	15	62.480	22.037	-0.803	1.00	30.76	CPS2
ATOM	1041	CG2	ILE	15	63.314	21.002	-0.056	1.00	29.83	CPS2
ATOM	1042	CG1	ILE	15	62.940	23.441	-0.407	1.00	29.97	CPS2
ATOM	1043	CD1	ILE	15	64.431	23.685	-0.657	1.00	30.60	CPS2
ATOM	1044	C	ILE	15	62.397	20.369	-2.673	1.00	33.28	CPS2
ATOM	1045	O	ILE	15	63.338	19.604	-2.900	1.00	33.51	CPS2
ATOM	1046	N	ALA	16	61.133	19.974	-2.712	1.00	34.78	CPS2
ATOM	1047	CA	ALA	16	60.789	18.597	-3.039	1.00	37.29	CPS2
ATOM	1048	CB	ALA	16	59.285	18.395	-2.921	1.00	36.48	CPS2
ATOM	1049	C	ALA	16	61.264	18.286	-4.459	1.00	39.28	CPS2
ATOM	1050	O	ALA	16	61.839	17.230	-4.716	1.00	40.75	CPS2
ATOM	1051	N	SER	17	61.034	19.219	-5.375	1.00	40.88	CPS2
ATOM	1052	CA	SER	17	61.439	19.046	-6.763	1.00	43.46	CPS2
ATOM	1053	CB	SER	17	61.012	20.261	-7.588	1.00	44.13	CPS2
ATOM	1054	OG	SER	17	61.450	20.150	-8.930	1.00	46.75	CPS2
ATOM	1055	C	SER	17	62.949	18.857	-6.866	1.00	44.93	CPS2
ATOM	1056	O	SER	17	63.432	18.058	-7.672	1.00	44.94	CPS2
ATOM	1057	N	MET	18	63.694	19.597	-6.052	1.00	45.72	CPS2
ATOM	1058	CA	MET	18	65.148	19.499	-6.060	1.00	47.01	CPS2
ATOM	1059	CB	MET	18	65.780	20.713	-5.374	1.00	47.40	CPS2
ATOM	1060	CG	MET	18	65.783	21.978	-6.201	1.00	48.61	CPS2
ATOM	1061	SD	MET	18	66.874	23.231	-5.488	1.00	51.56	CPS2
ATOM	1062	CE	MET	18	65.856	23.843	-4.148	1.00	49.70	CPS2
ATOM	1063	C	MET	18	65.637	18.233	-5.369	1.00	47.60	CPS2
ATOM	1064	O	MET	18	66.589	17.605	-5.822	1.00	48.05	CPS2
ATOM	1065	N	ALA	19	64.982	17.863	-4.275	1.00	48.91	CPS2
ATOM	1066	CA	ALA	19	65.365	16.682	-3.512	1.00	50.86	CPS2
ATOM	1067	CB	ALA	19	64.590	16.637	-2.209	1.00	50.39	CPS2
ATOM	1068	C	ALA	19	65.135	15.396	-4.296	1.00	53.04	CPS2
ATOM	1069	O	ALA	19	65.897	14.433	-4.171	1.00	52.81	CPS2
ATOM	1070	N	GLY	20	64.084	15.384	-5.108	1.00	54.91	CPS2
ATOM	1071	CA	GLY	20	63.773	14.201	-5.888	1.00	56.86	CPS2
ATOM	1072	C	GLY	20	64.693	13.980	-7.072	1.00	58.24	CPS2
ATOM	1073	O	GLY	20	65.285	12.909	-7.217	1.00	58.99	CPS2
ATOM	1074	N	ARG	21	64.827	14.996	-7.916	1.00	59.32	CPS2
ATOM	1075	CA	ARG	21	65.652	14.882	-9.107	1.00	60.71	CPS2
ATOM	1076	CB	ARG	21	65.279	15.975	-10.112	1.00	61.88	CPS2
ATOM	1077	CG	ARG	21	65.739	17.362	-9.716	1.00	63.83	CPS2
ATOM	1078	CD	ARG	21	65.818	18.274	-10.930	1.00	65.39	CPS2
ATOM	1079	NE	ARG	21	66.617	19.471	-10.669	1.00	67.17	CPS2
ATOM	1080	CZ	ARG	21	66.250	20.467	-9.867	1.00	67.54	CPS2
ATOM	1081	NH1	ARG	21	65.082	20.423	-9.237	1.00	68.19	CPS2
ATOM	1082	NH2	ARG	21	67.057	21.507	-9.693	1.00	67.30	CPS2

FIG. 1A-19

ATOM	1083	C	ARG	21	67.153	14.932	-8.857	1.00	61.11	CPS2
ATOM	1084	O	ARG	21	67.942	14.571	-9.735	1.00	61.28	CPS2
ATOM	1085	N	GLN	22	67.564	15.375	-7.674	1.00	61.25	CPS2
ATOM	1086	CA	GLN	22	68.994	15.461	-7.402	1.00	60.88	CPS2
ATOM	1087	CB	GLN	22	69.340	16.826	-6.795	1.00	61.70	CPS2
ATOM	1088	CG	GLN	22	69.033	17.998	-7.722	1.00	62.47	CPS2
ATOM	1089	CD	GLN	22	69.522	19.331	-7.180	1.00	63.25	CPS2
ATOM	1090	OE1	GLN	22	69.279	20.381	-7.779	1.00	63.34	CPS2
ATOM	1091	NE2	GLN	22	70.218	19.297	-6.047	1.00	63.02	CPS2
ATOM	1092	C	GLN	22	69.563	14.351	-6.530	1.00	60.08	CPS2
ATOM	1093	O	GLN	22	68.836	13.608	-5.867	1.00	60.33	CPS2
ATOM	1094	N	LYS	23	70.886	14.253	-6.569	1.00	59.12	CPS2
ATOM	1095	CA	LYS	23	71.665	13.273	-5.823	1.00	57.97	CPS2
ATOM	1096	CB	LYS	23	73.137	13.684	-5.890	1.00	59.44	CPS2
ATOM	1097	CG	LYS	23	73.362	15.214	-5.851	1.00	60.21	CPS2
ATOM	1098	CD	LYS	23	73.057	15.850	-4.501	1.00	59.91	CPS2
ATOM	1099	CE	LYS	23	73.391	17.340	-4.455	1.00	60.70	CPS2
ATOM	1100	NZ	LYS	23	72.466	18.181	-5.268	1.00	59.44	CPS2
ATOM	1101	C	LYS	23	71.253	13.118	-4.360	1.00	56.31	CPS2
ATOM	1102	O	LYS	23	70.226	12.517	-4.027	1.00	57.13	CPS2
ATOM	1103	N	ARG	24	72.112	13.635	-3.496	1.00	53.19	CPS2
ATOM	1104	CA	ARG	24	71.909	13.629	-2.062	1.00	50.41	CPS2
ATOM	1105	CB	ARG	24	73.117	12.987	-1.365	1.00	51.60	CPS2
ATOM	1106	CG	ARG	24	74.311	12.739	-2.286	1.00	51.97	CPS2
ATOM	1107	CD	ARG	24	75.442	12.014	-1.565	1.00	52.64	CPS2
ATOM	1108	NE	ARG	24	75.105	10.634	-1.218	1.00	51.83	CPS2
ATOM	1109	CZ	ARG	24	75.534	9.570	-1.892	1.00	51.87	CPS2
ATOM	1110	NH1	ARG	24	76.318	9.728	-2.950	1.00	51.30	CPS2
ATOM	1111	NH2	ARG	24	75.187	8.347	-1.505	1.00	51.09	CPS2
ATOM	1112	C	ARG	24	71.787	15.110	-1.717	1.00	47.01	CPS2
ATOM	1113	O	ARG	24	72.640	15.690	-1.043	1.00	46.57	CPS2
ATOM	1114	N	PHE	25	70.725	15.721	-2.238	1.00	42.31	CPS2
ATOM	1115	CA	PHE	25	70.450	17.134	-2.019	1.00	38.57	CPS2
ATOM	1116	CB	PHE	25	69.115	17.508	-2.679	1.00	37.72	CPS2
ATOM	1117	CG	PHE	25	68.680	18.926	-2.416	1.00	36.40	CPS2
ATOM	1118	CD1	PHE	25	67.682	19.202	-1.485	1.00	36.71	CPS2
ATOM	1119	CD2	PHE	25	69.285	19.986	-3.080	1.00	37.10	CPS2
ATOM	1120	CE1	PHE	25	67.297	20.518	-1.220	1.00	36.02	CPS2
ATOM	1121	CE2	PHE	25	68.910	21.305	-2.824	1.00	35.88	CPS2
ATOM	1122	CZ	PHE	25	67.914	21.572	-1.891	1.00	36.06	CPS2
ATOM	1123	C	PHE	25	70.415	17.465	-0.528	1.00	36.15	CPS2
ATOM	1124	O	PHE	25	71.053	18.423	-0.079	1.00	35.69	CPS2
ATOM	1125	N	ALA	26	69.671	16.664	0.228	1.00	33.10	CPS2
ATOM	1126	CA	ALA	26	69.548	16.865	1.667	1.00	32.04	CPS2
ATOM	1127	CB	ALA	26	68.663	15.780	2.270	1.00	30.86	CPS2
ATOM	1128	C	ALA	26	70.931	16.835	2.312	1.00	31.57	CPS2
ATOM	1129	O	ALA	26	71.249	17.655	3.180	1.00	28.07	CPS2
ATOM	1130	N	GLU	27	71.747	15.881	1.868	1.00	29.98	CPS2
ATOM	1131	CA	GLU	27	73.102	15.717	2.382	1.00	30.25	CPS2
ATOM	1132	CB	GLU	27	73.745	14.457	1.794	1.00	31.17	CPS2
ATOM	1133	CG	GLU	27	73.219	13.134	2.356	1.00	35.24	CPS2
ATOM	1134	CD	GLU	27	71.772	12.823	1.978	1.00	37.65	CPS2
ATOM	1135	OE1	GLU	27	71.300	13.296	0.918	1.00	38.95	CPS2
ATOM	1136	OE2	GLU	27	71.113	12.076	2.742	1.00	40.73	CPS2
ATOM	1137	C	GLU	27	73.974	16.925	2.063	1.00	28.88	CPS2
ATOM	1138	O	GLU	27	74.879	17.254	2.823	1.00	28.66	CPS2
ATOM	1139	N	ARG	28	73.705	17.578	0.935	1.00	27.77	CPS2

FIG. 1A-20

ATOM	1140	CA	ARG	28	74.470	18.754	0.532	1.00	29.47	CPS2
ATOM	1141	CB	ARG	28	74.201	19.076	-0.948	1.00	30.98	CPS2
ATOM	1142	CG	ARG	28	74.785	20.407	-1.424	1.00	35.00	CPS2
ATOM	1143	CD	ARG	28	74.806	20.528	-2.953	1.00	38.43	CPS2
ATOM	1144	NE	ARG	28	73.480	20.654	-3.557	1.00	40.71	CPS2
ATOM	1145	CZ	ARG	28	72.809	21.797	-3.683	1.00	42.27	CPS2
ATOM	1146	NH1	ARG	28	73.327	22.940	-3.248	1.00	42.45	CPS2
ATOM	1147	NH2	ARG	28	71.613	21.798	-4.259	1.00	44.17	CPS2
ATOM	1148	C	ARG	28	74.137	19.987	1.387	1.00	28.50	CPS2
ATOM	1149	O	ARG	28	75.003	20.811	1.669	1.00	29.58	CPS2
ATOM	1150	N	ILE	29	72.879	20.105	1.788	1.00	26.47	CPS2
ATOM	1151	CA	ILE	29	72.426	21.256	2.570	1.00	26.32	CPS2
ATOM	1152	CB	ILE	29	70.908	21.475	2.389	1.00	25.79	CPS2
ATOM	1153	CG2	ILE	29	70.467	22.729	3.147	1.00	24.32	CPS2
ATOM	1154	CG1	ILE	29	70.559	21.566	0.902	1.00	23.95	CPS2
ATOM	1155	CD1	ILE	29	71.283	22.665	0.158	1.00	26.12	CPS2
ATOM	1156	C	ILE	29	72.681	21.128	4.064	1.00	26.65	CPS2
ATOM	1157	O	ILE	29	73.024	22.110	4.739	1.00	26.47	CPS2
ATOM	1158	N	LEU	30	72.516	19.908	4.566	1.00	26.29	CPS2
ATOM	1159	CA	LEU	30	72.638	19.616	5.981	1.00	26.30	CPS2
ATOM	1160	CB	LEU	30	71.518	18.645	6.371	1.00	26.05	CPS2
ATOM	1161	CG	LEU	30	70.095	19.059	5.957	1.00	26.30	CPS2
ATOM	1162	CD1	LEU	30	69.081	18.002	6.387	1.00	26.56	CPS2
ATOM	1163	CD2	LEU	30	69.762	20.400	6.602	1.00	24.24	CPS2
ATOM	1164	C	LEU	30	73.972	19.075	6.497	1.00	27.26	CPS2
ATOM	1165	O	LEU	30	74.731	18.419	5.771	1.00	28.28	CPS2
ATOM	1166	N	THR	31	74.246	19.372	7.765	1.00	26.23	CPS2
ATOM	1167	CA	THR	31	75.451	18.898	8.434	1.00	26.09	CPS2
ATOM	1168	CB	THR	31	75.844	19.806	9.627	1.00	24.78	CPS2
ATOM	1169	OG1	THR	31	74.834	19.723	10.638	1.00	25.44	CPS2
ATOM	1170	CG2	THR	31	75.998	21.253	9.172	1.00	25.52	CPS2
ATOM	1171	C	THR	31	75.106	17.516	8.978	1.00	26.34	CPS2
ATOM	1172	O	THR	31	73.945	17.106	8.956	1.00	25.24	CPS2
ATOM	1173	N	ARG	32	76.108	16.791	9.463	1.00	28.14	CPS2
ATOM	1174	CA	ARG	32	75.872	15.456	10.005	1.00	30.16	CPS2
ATOM	1175	CB	ARG	32	77.195	14.862	10.519	1.00	32.90	CPS2
ATOM	1176	CG	ARG	32	77.070	13.518	11.243	1.00	37.77	CPS2
ATOM	1177	CD	ARG	32	78.452	13.018	11.667	1.00	42.29	CPS2
ATOM	1178	NE	ARG	32	78.428	12.082	12.796	1.00	46.64	CPS2
ATOM	1179	CZ	ARG	32	78.020	10.817	12.728	1.00	48.51	CPS2
ATOM	1180	NH1	ARG	32	77.588	10.314	11.581	1.00	50.24	CPS2
ATOM	1181	NH2	ARG	32	78.058	10.045	13.809	1.00	49.25	CPS2
ATOM	1182	C	ARG	32	74.812	15.450	11.116	1.00	29.69	CPS2
ATOM	1183	O	ARG	32	73.946	14.577	11.149	1.00	29.33	CPS2
ATOM	1184	N	SER	33	74.858	16.428	12.019	1.00	29.98	CPS2
ATOM	1185	CA	SER	33	73.886	16.473	13.112	1.00	29.46	CPS2
ATOM	1186	CB	SER	33	74.338	17.475	14.180	1.00	32.61	CPS2
ATOM	1187	OG	SER	33	74.402	18.784	13.645	1.00	37.61	CPS2
ATOM	1188	C	SER	33	72.464	16.813	12.652	1.00	28.59	CPS2
ATOM	1189	O	SER	33	71.488	16.317	13.211	1.00	27.50	CPS2
ATOM	1190	N	GLU	34	72.345	17.682	11.654	1.00	27.39	CPS2
ATOM	1191	CA	GLU	34	71.036	18.051	11.131	1.00	27.27	CPS2
ATOM	1192	CB	GLU	34	71.178	19.215	10.140	1.00	26.09	CPS2
ATOM	1193	CG	GLU	34	71.493	20.554	10.824	1.00	27.08	CPS2
ATOM	1194	CD	GLU	34	71.939	21.642	9.860	1.00	27.39	CPS2
ATOM	1195	OE1	GLU	34	71.813	22.838	10.220	1.00	26.38	CPS2
ATOM	1196	OE2	GLU	34	72.427	21.310	8.755	1.00	25.66	CPS2

FIG. 1A-21

ATOM	1197	C	GLU	34	70.443	16.828	10.437	1.00 27.36	CPS2
ATOM	1198	O	GLU	34	69.239	16.562	10.532	1.00 26.33	CPS2
ATOM	1199	N	LEU	35	71.302	16.077	9.750	1.00 28.28	CPS2
ATOM	1200	CA	LEU	35	70.862	14.877	9.045	1.00 29.11	CPS2
ATOM	1201	CB	LEU	35	72.021	14.251	8.270	1.00 28.46	CPS2
ATOM	1202	CG	LEU	35	72.336	14.922	6.940	1.00 27.65	CPS2
ATOM	1203	CD1	LEU	35	73.659	14.380	6.379	1.00 29.47	CPS2
ATOM	1204	CD2	LEU	35	71.182	14.664	5.965	1.00 28.02	CPS2
ATOM	1205	C	LEU	35	70.281	13.851	9.998	1.00 30.80	CPS2
ATOM	1206	O	LEU	35	69.303	13.191	9.668	1.00 31.95	CPS2
ATOM	1207	N	ASP	36	70.883	13.709	11.175	1.00 32.92	CPS2
ATOM	1208	CA	ASP	36	70.380	12.756	12.161	1.00 35.31	CPS2
ATOM	1209	CB	ASP	36	71.247	12.759	13.416	1.00 38.59	CPS2
ATOM	1210	CG	ASP	36	72.527	11.974	13.236	1.00 43.41	CPS2
ATOM	1211	OD1	ASP	36	72.449	10.838	12.713	1.00 47.13	CPS2
ATOM	1212	OD2	ASP	36	73.606	12.480	13.618	1.00 45.83	CPS2
ATOM	1213	C	ASP	36	68.948	13.107	12.531	1.00 35.32	CPS2
ATOM	1214	O	ASP	36	68.108	12.228	12.733	1.00 35.28	CPS2
ATOM	1215	N	GLN	37	68.675	14.404	12.621	1.00 34.28	CPS2
ATOM	1216	CA	GLN	37	67.338	14.881	12.945	1.00 32.79	CPS2
ATOM	1217	CB	GLN	37	67.401	16.378	13.297	1.00 33.92	CPS2
ATOM	1218	CG	GLN	37	68.022	16.651	14.662	1.00 35.15	CPS2
ATOM	1219	CD	GLN	37	68.443	18.110	14.876	1.00 36.52	CPS2
ATOM	1220	OE1	GLN	37	68.733	18.517	16.001	1.00 37.53	CPS2
ATOM	1221	NE2	GLN	37	68.495	18.887	13.799	1.00 34.94	CPS2
ATOM	1222	C	GLN	37	66.431	14.645	11.733	1.00 32.14	CPS2
ATOM	1223	O	GLN	37	65.284	14.214	11.863	1.00 31.52	CPS2
ATOM	1224	N	TYR	38	66.971	14.914	10.552	1.00 30.64	CPS2
ATOM	1225	CA	TYR	38	66.239	14.753	9.307	1.00 30.51	CPS2
ATOM	1226	CB	TYR	38	67.112	15.245	8.148	1.00 29.87	CPS2
ATOM	1227	CG	TYR	38	66.544	15.040	6.762	1.00 30.29	CPS2
ATOM	1228	CD1	TYR	38	66.975	13.983	5.957	1.00 31.01	CPS2
ATOM	1229	CE1	TYR	38	66.500	13.829	4.653	1.00 31.49	CPS2
ATOM	1230	CD2	TYR	38	65.614	15.935	6.231	1.00 30.83	CPS2
ATOM	1231	CE2	TYR	38	65.135	15.792	4.938	1.00 31.82	CPS2
ATOM	1232	CZ	TYR	38	65.582	14.742	4.153	1.00 32.74	CPS2
ATOM	1233	OH	TYR	38	65.116	14.623	2.868	1.00 33.33	CPS2
ATOM	1234	C	TYR	38	65.802	13.308	9.064	1.00 31.79	CPS2
ATOM	1235	O	TYR	38	64.631	13.048	8.773	1.00 30.55	CPS2
ATOM	1236	N	TYR	39	66.739	12.372	9.190	1.00 31.62	CPS2
ATOM	1237	CA	TYR	39	66.423	10.965	8.946	1.00 33.46	CPS2
ATOM	1238	CB	TYR	39	67.675	10.096	9.077	1.00 31.46	CPS2
ATOM	1239	CG	TYR	39	68.760	10.350	8.045	1.00 30.99	CPS2
ATOM	1240	CD1	TYR	39	68.449	10.548	6.702	1.00 31.00	CPS2
ATOM	1241	CE1	TYR	39	69.458	10.707	5.744	1.00 31.73	CPS2
ATOM	1242	CD2	TYR	39	70.108	10.321	8.413	1.00 32.22	CPS2
ATOM	1243	CE2	TYR	39	71.125	10.474	7.468	1.00 32.57	CPS2
ATOM	1244	CZ	TYR	39	70.795	10.665	6.137	1.00 32.96	CPS2
ATOM	1245	OH	TYR	39	71.813	10.784	5.211	1.00 33.59	CPS2
ATOM	1246	C	TYR	39	65.331	10.411	9.862	1.00 34.30	CPS2
ATOM	1247	O	TYR	39	64.653	9.451	9.506	1.00 35.26	CPS2
ATOM	1248	N	GLU	40	65.155	11.015	11.030	1.00 36.00	CPS2
ATOM	1249	CA	GLU	40	64.144	10.555	11.980	1.00 38.47	CPS2
ATOM	1250	CB	GLU	40	64.468	11.069	13.387	1.00 41.11	CPS2
ATOM	1251	CG	GLU	40	65.650	10.394	14.052	1.00 46.35	CPS2
ATOM	1252	CD	GLU	40	65.427	8.903	14.247	1.00 49.30	CPS2
ATOM	1253	OE1	GLU	40	64.505	8.527	15.006	1.00 50.90	CPS2

FIG. 1A-22

ATOM	1254	OE2	GLU	40	66.174	8.108	13.632	1.00	51.72	CPS2
ATOM	1255	C	GLU	40	62.720	10.980	11.631	1.00	38.59	CPS2
ATOM	1256	O	GLU	40	61.761	10.472	12.210	1.00	38.70	CPS2
ATOM	1257	N	LEU	41	62.579	11.905	10.688	1.00	37.33	CPS2
ATOM	1258	CA	LEU	41	61.262	12.409	10.318	1.00	37.21	CPS2
ATOM	1259	CB	LEU	41	61.371	13.881	9.908	1.00	36.12	CPS2
ATOM	1260	CG	LEU	41	61.978	14.843	10.928	1.00	35.44	CPS2
ATOM	1261	CD1	LEU	41	62.095	16.224	10.296	1.00	35.33	CPS2
ATOM	1262	CD2	LEU	41	61.110	14.897	12.175	1.00	36.15	CPS2
ATOM	1263	C	LEU	41	60.540	11.653	9.210	1.00	37.79	CPS2
ATOM	1264	O	LEU	41	61.147	10.905	8.441	1.00	37.84	CPS2
ATOM	1265	N	SER	42	59.231	11.882	9.130	1.00	38.99	CPS2
ATOM	1266	CA	SER	42	58.394	11.272	8.105	1.00	39.66	CPS2
ATOM	1267	CB	SER	42	56.916	11.461	8.451	1.00	40.41	CPS2
ATOM	1268	OG	SER	42	56.529	12.813	8.277	1.00	40.55	CPS2
ATOM	1269	C	SER	42	58.688	11.947	6.769	1.00	40.88	CPS2
ATOM	1270	O	SER	42	59.404	12.948	6.716	1.00	40.22	CPS2
ATOM	1271	N	GLU	43	58.118	11.405	5.698	1.00	41.38	CPS2
ATOM	1272	CA	GLU	43	58.310	11.948	4.358	1.00	41.99	CPS2
ATOM	1273	CB	GLU	43	57.466	11.173	3.340	1.00	44.33	CPS2
ATOM	1274	CG	GLU	43	56.922	9.822	3.821	1.00	47.83	CPS2
ATOM	1275	CD	GLU	43	55.963	9.946	5.005	1.00	50.30	CPS2
ATOM	1276	OE1	GLU	43	55.186	10.935	5.055	1.00	50.62	CPS2
ATOM	1277	OE2	GLU	43	55.982	9.045	5.877	1.00	48.97	CPS2
ATOM	1278	C	GLU	43	57.921	13.425	4.294	1.00	40.64	CPS2
ATOM	1279	O	GLU	43	58.662	14.259	3.767	1.00	40.30	CPS2
ATOM	1280	N	LYS	44	56.747	13.739	4.825	1.00	39.19	CPS2
ATOM	1281	CA	LYS	44	56.249	15.112	4.821	1.00	39.31	CPS2
ATOM	1282	CB	LYS	44	54.787	15.140	5.269	1.00	40.00	CPS2
ATOM	1283	CG	LYS	44	54.112	16.491	5.107	1.00	42.53	CPS2
ATOM	1284	CD	LYS	44	52.721	16.472	5.719	1.00	44.55	CPS2
ATOM	1285	CE	LYS	44	52.031	17.817	5.592	1.00	45.48	CPS2
ATOM	1286	NZ	LYS	44	50.783	17.861	6.406	1.00	47.64	CPS2
ATOM	1287	C	LYS	44	57.075	16.023	5.732	1.00	38.50	CPS2
ATOM	1288	O	LYS	44	57.446	17.136	5.345	1.00	38.08	CPS2
ATOM	1289	N	ARG	45	57.345	15.554	6.947	1.00	36.81	CPS2
ATOM	1290	CA	ARG	45	58.125	16.335	7.898	1.00	36.28	CPS2
ATOM	1291	CB	ARG	45	58.162	15.624	9.254	1.00	37.98	CPS2
ATOM	1292	CG	ARG	45	56.911	15.843	10.106	1.00	41.93	CPS2
ATOM	1293	CD	ARG	45	57.135	16.960	11.117	1.00	45.38	CPS2
ATOM	1294	NE	ARG	45	57.655	18.160	10.468	1.00	49.29	CPS2
ATOM	1295	CZ	ARG	45	58.565	18.968	11.002	1.00	49.81	CPS2
ATOM	1296	NH1	ARG	45	59.064	18.714	12.206	1.00	51.08	CPS2
ATOM	1297	NH2	ARG	45	58.993	20.022	10.323	1.00	50.35	CPS2
ATOM	1298	C	ARG	45	59.537	16.595	7.382	1.00	34.46	CPS2
ATOM	1299	O	ARG	45	60.105	17.657	7.629	1.00	33.18	CPS2
ATOM	1300	N	LYS	46	60.107	15.630	6.662	1.00	32.44	CPS2
ATOM	1301	CA	LYS	46	61.444	15.814	6.110	1.00	32.32	CPS2
ATOM	1302	CB	LYS	46	61.891	14.589	5.295	1.00	32.49	CPS2
ATOM	1303	CG	LYS	46	62.375	13.419	6.133	1.00	33.28	CPS2
ATOM	1304	CD	LYS	46	62.872	12.296	5.245	1.00	34.31	CPS2
ATOM	1305	CE	LYS	46	63.389	11.131	6.065	1.00	35.44	CPS2
ATOM	1306	NZ	LYS	46	63.700	9.994	5.169	1.00	36.69	CPS2
ATOM	1307	C	LYS	46	61.479	17.039	5.206	1.00	31.46	CPS2
ATOM	1308	O	LYS	46	62.393	17.856	5.290	1.00	31.48	CPS2
ATOM	1309	N	ASN	47	60.481	17.163	4.336	1.00	30.42	CPS2
ATOM	1310	CA	ASN	47	60.417	18.286	3.407	1.00	31.16	CPS2

FIG. 1A-23

ATOM	1311	CB	ASN	47	59.240	18.101	2.437	1.00 32.45	CPS2
ATOM	1312	CG	ASN	47	59.080	19.269	1.470	1.00 34.97	CPS2
ATOM	1313	OD1	ASN	47	59.977	19.575	0.684	1.00 37.44	CPS2
ATOM	1314	ND2	ASN	47	57.928	19.923	1.525	1.00 35.87	CPS2
ATOM	1315	C	ASN	47	60.290	19.612	4.157	1.00 29.73	CPS2
ATOM	1316	O	ASN	47	60.946	20.587	3.803	1.00 28.79	CPS2
ATOM	1317	N	GLU	48	59.462	19.637	5.195	1.00 28.89	CPS2
ATOM	1318	CA	GLU	48	59.265	20.853	5.984	1.00 29.80	CPS2
ATOM	1319	CB	GLU	48	58.162	20.642	7.019	1.00 32.74	CPS2
ATOM	1320	CG	GLU	48	56.837	20.225	6.424	1.00 37.62	CPS2
ATOM	1321	CD	GLU	48	55.785	19.953	7.482	1.00 40.29	CPS2
ATOM	1322	OE1	GLU	48	54.683	19.506	7.113	1.00 41.90	CPS2
ATOM	1323	OE2	GLU	48	56.059	20.193	8.679	1.00 42.74	CPS2
ATOM	1324	C	GLU	48	60.554	21.231	6.700	1.00 28.72	CPS2
ATOM	1325	O	GLU	48	60.956	22.396	6.720	1.00 27.50	CPS2
ATOM	1326	N	PHE	49	61.192	20.230	7.296	1.00 26.72	CPS2
ATOM	1327	CA	PHE	49	62.432	20.433	8.023	1.00 26.17	CPS2
ATOM	1328	CB	PHE	49	62.877	19.116	8.665	1.00 27.12	CPS2
ATOM	1329	CG	PHE	49	64.186	19.205	9.397	1.00 26.24	CPS2
ATOM	1330	CD1	PHE	49	64.219	19.514	10.750	1.00 27.02	CPS2
ATOM	1331	CD2	PHE	49	65.385	18.967	8.734	1.00 28.35	CPS2
ATOM	1332	CE1	PHE	49	65.429	19.578	11.436	1.00 27.13	CPS2
ATOM	1333	CE2	PHE	49	66.603	19.030	9.411	1.00 27.87	CPS2
ATOM	1334	CZ	PHE	49	66.615	19.336	10.770	1.00 27.13	CPS2
ATOM	1335	C	PHE	49	63.522	20.935	7.091	1.00 24.61	CPS2
ATOM	1336	O	PHE	49	64.208	21.907	7.390	1.00 24.60	CPS2
ATOM	1337	N	LEU	50	63.685	20.266	5.957	1.00 23.67	CPS2
ATOM	1338	CA	LEU	50	64.710	20.650	5.000	1.00 23.23	CPS2
ATOM	1339	CB	LEU	50	64.763	19.626	3.862	1.00 24.17	CPS2
ATOM	1340	CG	LEU	50	65.810	19.767	2.758	1.00 26.00	CPS2
ATOM	1341	CD1	LEU	50	67.217	19.817	3.351	1.00 25.89	CPS2
ATOM	1342	CD2	LEU	50	65.685	18.570	1.810	1.00 26.96	CPS2
ATOM	1343	C	LEU	50	64.465	22.053	4.448	1.00 23.30	CPS2
ATOM	1344	O	LEU	50	65.391	22.849	4.317	1.00 22.85	CPS2
ATOM	1345	N	ALA	51	63.218	22.366	4.127	1.00 21.99	CPS2
ATOM	1346	CA	ALA	51	62.914	23.684	3.586	1.00 21.37	CPS2
ATOM	1347	CB	ALA	51	61.438	23.766	3.206	1.00 19.49	CPS2
ATOM	1348	C	ALA	51	63.262	24.772	4.610	1.00 19.95	CPS2
ATOM	1349	O	ALA	51	63.812	25.815	4.252	1.00 19.91	CPS2
ATOM	1350	N	GLY	52	62.943	24.508	5.871	1.00 20.32	CPS2
ATOM	1351	CA	GLY	52	63.207	25.466	6.939	1.00 20.53	CPS2
ATOM	1352	C	GLY	52	64.690	25.678	7.161	1.00 21.59	CPS2
ATOM	1353	O	GLY	52	65.140	26.823	7.292	1.00 20.12	CPS2
ATOM	1354	N	ARG	53	65.452	24.581	7.211	1.00 20.75	CPS2
ATOM	1355	CA	ARG	53	66.900	24.681	7.405	1.00 21.49	CPS2
ATOM	1356	CB	ARG	53	67.511	23.289	7.639	1.00 20.94	CPS2
ATOM	1357	CG	ARG	53	67.662	22.904	9.121	1.00 21.90	CPS2
ATOM	1358	CD	ARG	53	66.357	23.082	9.905	1.00 23.39	CPS2
ATOM	1359	NE	ARG	53	66.538	22.829	11.335	1.00 24.30	CPS2
ATOM	1360	CZ	ARG	53	65.666	23.195	12.272	1.00 25.08	CPS2
ATOM	1361	NH1	ARG	53	64.548	23.827	11.934	1.00 25.43	CPS2
ATOM	1362	NH2	ARG	53	65.921	22.959	13.551	1.00 26.80	CPS2
ATOM	1363	C	ARG	53	67.541	25.359	6.201	1.00 20.90	CPS2
ATOM	1364	O	ARG	53	68.447	26.176	6.353	1.00 20.27	CPS2
ATOM	1365	N	PHE	54	67.069	25.021	5.002	1.00 20.29	CPS2
ATOM	1366	CA	PHE	54	67.583	25.631	3.779	1.00 21.05	CPS2
ATOM	1367	CB	PHE	54	66.889	24.996	2.550	1.00 21.38	CPS2

FIG. 1A-24

ATOM	1368	CG	PHE	54	67.310	25.573	1.218	1.00	22.85	CPS2
ATOM	1369	CD1	PHE	54	66.623	26.646	0.660	1.00	23.51	CPS2
ATOM	1370	CD2	PHE	54	68.363	25.008	0.495	1.00	23.11	CPS2
ATOM	1371	CE1	PHE	54	66.970	27.148	-0.600	1.00	23.62	CPS2
ATOM	1372	CE2	PHE	54	68.716	25.499	-0.761	1.00	24.74	CPS2
ATOM	1373	CZ	PHE	54	68.015	26.575	-1.313	1.00	24.84	CPS2
ATOM	1374	C	PHE	54	67.334	27.144	3.823	1.00	20.71	CPS2
ATOM	1375	O	PHE	54	68.225	27.939	3.523	1.00	20.44	CPS2
ATOM	1376	N	ALA	55	66.118	27.542	4.191	1.00	20.38	CPS2
ATOM	1377	CA	ALA	55	65.772	28.967	4.268	1.00	20.18	CPS2
ATOM	1378	CB	ALA	55	64.299	29.138	4.665	1.00	19.50	CPS2
ATOM	1379	C	ALA	55	66.654	29.701	5.276	1.00	20.15	CPS2
ATOM	1380	O	ALA	55	67.111	30.822	5.021	1.00	19.68	CPS2
ATOM	1381	N	ALA	56	66.872	29.071	6.428	1.00	20.22	CPS2
ATOM	1382	CA	ALA	56	67.706	29.657	7.476	1.00	19.63	CPS2
ATOM	1383	CB	ALA	56	67.670	28.772	8.737	1.00	20.93	CPS2
ATOM	1384	C	ALA	56	69.152	29.841	7.014	1.00	20.43	CPS2
ATOM	1385	O	ALA	56	69.780	30.869	7.307	1.00	19.00	CPS2
ATOM	1386	N	LYS	57	69.702	28.840	6.322	1.00	19.36	CPS2
ATOM	1387	CA	LYS	57	71.084	28.955	5.858	1.00	19.89	CPS2
ATOM	1388	CB	LYS	57	71.622	27.598	5.388	1.00	19.91	CPS2
ATOM	1389	CG	LYS	57	71.595	26.550	6.501	1.00	20.56	CPS2
ATOM	1390	CD	LYS	57	72.389	25.285	6.150	1.00	21.63	CPS2
ATOM	1391	CE	LYS	57	72.426	24.334	7.358	1.00	20.15	CPS2
ATOM	1392	NZ	LYS	57	73.457	23.262	7.208	1.00	19.99	CPS2
ATOM	1393	C	LYS	57	71.176	29.993	4.754	1.00	19.82	CPS2
ATOM	1394	O	LYS	57	72.136	30.755	4.698	1.00	20.57	CPS2
ATOM	1395	N	GLU	58	70.179	30.036	3.871	1.00	18.71	CPS2
ATOM	1396	CA	GLU	58	70.187	31.045	2.822	1.00	20.25	CPS2
ATOM	1397	CB	GLU	58	68.993	30.868	1.870	1.00	23.44	CPS2
ATOM	1398	CG	GLU	58	69.120	29.710	0.871	1.00	28.15	CPS2
ATOM	1399	CD	GLU	58	70.261	29.896	-0.124	1.00	31.42	CPS2
ATOM	1400	OE1	GLU	58	70.713	31.042	-0.335	1.00	33.78	CPS2
ATOM	1401	OE2	GLU	58	70.701	28.891	-0.713	1.00	35.13	CPS2
ATOM	1402	C	GLU	58	70.116	32.436	3.477	1.00	20.06	CPS2
ATOM	1403	O	GLU	58	70.878	33.335	3.117	1.00	20.02	CPS2
ATOM	1404	N	ALA	59	69.203	32.611	4.433	1.00	18.56	CPS2
ATOM	1405	CA	ALA	59	69.066	33.901	5.107	1.00	19.36	CPS2
ATOM	1406	CB	ALA	59	67.919	33.853	6.142	1.00	18.28	CPS2
ATOM	1407	C	ALA	59	70.388	34.280	5.789	1.00	19.60	CPS2
ATOM	1408	O	ALA	59	70.833	35.429	5.712	1.00	20.42	CPS2
ATOM	1409	N	PHE	60	71.016	33.314	6.452	1.00	18.99	CPS2
ATOM	1410	CA	PHE	60	72.284	33.591	7.119	1.00	19.29	CPS2
ATOM	1411	CB	PHE	60	72.790	32.350	7.862	1.00	20.46	CPS2
ATOM	1412	CG	PHE	60	74.128	32.555	8.501	1.00	21.05	CPS2
ATOM	1413	CD1	PHE	60	74.225	33.085	9.785	1.00	21.57	CPS2
ATOM	1414	CD2	PHE	60	75.297	32.313	7.783	1.00	23.12	CPS2
ATOM	1415	CE1	PHE	60	75.476	33.377	10.343	1.00	22.68	CPS2
ATOM	1416	CE2	PHE	60	76.554	32.605	8.332	1.00	22.55	CPS2
ATOM	1417	CZ	PHE	60	76.638	33.136	9.610	1.00	22.82	CPS2
ATOM	1418	C	PHE	60	73.338	34.020	6.092	1.00	20.21	CPS2
ATOM	1419	O	PHE	60	74.089	34.965	6.320	1.00	19.97	CPS2
ATOM	1420	N	SER	61	73.396	33.318	4.960	1.00	20.80	CPS2
ATOM	1421	CA	SER	61	74.372	33.641	3.920	1.00	20.87	CPS2
ATOM	1422	CB	SER	61	74.287	32.633	2.762	1.00	21.27	CPS2
ATOM	1423	OG	SER	61	73.161	32.874	1.942	1.00	22.46	CPS2
ATOM	1424	C	SER	61	74.190	35.058	3.389	1.00	21.75	CPS2

FIG. 1A-25

ATOM	1425	O	SER	61	75.161	35.709	2.981	1.00	22.83	CPS2
ATOM	1426	N	LYS	62	72.949	35.541	3.396	1.00	20.78	CPS2
ATOM	1427	CA	LYS	62	72.657	36.890	2.934	1.00	21.54	CPS2
ATOM	1428	CB	LYS	62	71.158	37.027	2.627	1.00	22.99	CPS2
ATOM	1429	CG	LYS	62	70.696	36.164	1.444	1.00	27.37	CPS2
ATOM	1430	CD	LYS	62	69.195	35.912	1.505	1.00	30.44	CPS2
ATOM	1431	CE	LYS	62	68.439	36.617	0.401	1.00	33.74	CPS2
ATOM	1432	NZ	LYS	62	68.581	35.960	-0.917	1.00	35.02	CPS2
ATOM	1433	C	LYS	62	73.084	37.922	3.985	1.00	22.13	CPS2
ATOM	1434	O	LYS	62	73.546	39.009	3.638	1.00	22.23	CPS2
ATOM	1435	N	ALA	63	72.929	37.581	5.264	1.00	21.23	CPS2
ATOM	1436	CA	ALA	63	73.329	38.488	6.335	1.00	20.30	CPS2
ATOM	1437	CB	ALA	63	72.813	37.988	7.694	1.00	21.99	CPS2
ATOM	1438	C	ALA	63	74.851	38.541	6.337	1.00	22.63	CPS2
ATOM	1439	O	ALA	63	75.439	39.604	6.541	1.00	22.47	CPS2
ATOM	1440	N	PHE	64	75.473	37.387	6.092	1.00	23.43	CPS2
ATOM	1441	CA	PHE	64	76.934	37.257	6.040	1.00	26.03	CPS2
ATOM	1442	CB	PHE	64	77.315	35.788	5.814	1.00	28.19	CPS2
ATOM	1443	CG	PHE	64	78.780	35.482	6.042	1.00	31.14	CPS2
ATOM	1444	CD1	PHE	64	79.301	35.418	7.329	1.00	33.14	CPS2
ATOM	1445	CD2	PHE	64	79.624	35.224	4.965	1.00	32.47	CPS2
ATOM	1446	CE1	PHE	64	80.652	35.094	7.545	1.00	34.43	CPS2
ATOM	1447	CE2	PHE	64	80.969	34.900	5.163	1.00	33.63	CPS2
ATOM	1448	CZ	PHE	64	81.484	34.834	6.457	1.00	33.53	CPS2
ATOM	1449	C	PHE	64	77.481	38.136	4.905	1.00	27.97	CPS2
ATOM	1450	O	PHE	64	78.645	38.549	4.935	1.00	29.10	CPS2
ATOM	1451	N	GLY	65	76.642	38.388	3.901	1.00	28.14	CPS2
ATOM	1452	CA	GLY	65	76.999	39.256	2.786	1.00	29.01	CPS2
ATOM	1453	C	GLY	65	77.588	38.652	1.523	1.00	30.18	CPS2
ATOM	1454	O	GLY	65	77.945	39.377	0.596	1.00	31.12	CPS2
ATOM	1455	N	THR	66	77.660	37.332	1.454	1.00	30.26	CPS2
ATOM	1456	CA	THR	66	78.268	36.684	0.302	1.00	30.90	CPS2
ATOM	1457	CB	THR	66	79.499	35.898	0.744	1.00	30.61	CPS2
ATOM	1458	OG1	THR	66	79.078	34.838	1.607	1.00	32.42	CPS2
ATOM	1459	CG2	THR	66	80.457	36.790	1.525	1.00	31.71	CPS2
ATOM	1460	C	THR	66	77.362	35.697	-0.410	1.00	31.06	CPS2
ATOM	1461	O	THR	66	77.601	35.355	-1.573	1.00	32.11	CPS2
ATOM	1462	N	GLY	67	76.332	35.232	0.288	1.00	30.08	CPS2
ATOM	1463	CA	GLY	67	75.460	34.226	-0.285	1.00	29.32	CPS2
ATOM	1464	C	GLY	67	76.230	32.923	-0.146	1.00	29.07	CPS2
ATOM	1465	O	GLY	67	77.357	32.929	0.354	1.00	28.18	CPS2
ATOM	1466	N	ILE	68	75.640	31.809	-0.566	1.00	29.24	CPS2
ATOM	1467	CA	ILE	68	76.315	30.518	-0.477	1.00	30.11	CPS2
ATOM	1468	CB	ILE	68	75.293	29.347	-0.467	1.00	29.33	CPS2
ATOM	1469	CG2	ILE	68	76.018	28.010	-0.446	1.00	29.51	CPS2
ATOM	1470	CG1	ILE	68	74.388	29.434	0.769	1.00	28.22	CPS2
ATOM	1471	CD1	ILE	68	75.100	29.195	2.089	1.00	25.10	CPS2
ATOM	1472	C	ILE	68	77.237	30.385	-1.697	1.00	32.39	CPS2
ATOM	1473	O	ILE	68	76.831	30.654	-2.827	1.00	32.91	CPS2
ATOM	1474	N	GLY	69	78.476	29.979	-1.460	1.00	32.97	CPS2
ATOM	1475	CA	GLY	69	79.419	29.834	-2.552	1.00	35.33	CPS2
ATOM	1476	C	GLY	69	80.810	29.564	-2.028	1.00	36.14	CPS2
ATOM	1477	O	GLY	69	80.970	28.924	-0.992	1.00	36.01	CPS2
ATOM	1478	N	ALA	70	81.814	30.065	-2.742	1.00	37.62	CPS2
ATOM	1479	CA	ALA	70	83.212	29.872	-2.379	1.00	38.31	CPS2
ATOM	1480	CB	ALA	70	84.110	30.468	-3.473	1.00	38.64	CPS2
ATOM	1481	C	ALA	70	83.577	30.474	-1.025	1.00	38.65	CPS2

FIG. 1A-26

ATOM	1482	O	ALA	70	84.488	29.999	-0.345	1.00 39.72	CPS2
ATOM	1483	N	GLN	71	82.858	31.515	-0.628	1.00 38.67	CPS2
ATOM	1484	CA	GLN	71	83.130	32.197	0.630	1.00 37.32	CPS2
ATOM	1485	CB	GLN	71	82.744	33.666	0.472	1.00 40.43	CPS2
ATOM	1486	CG	GLN	71	83.693	34.659	1.118	1.00 44.57	CPS2
ATOM	1487	CD	GLN	71	83.654	36.018	0.431	1.00 46.06	CPS2
ATOM	1488	OE1	GLN	71	84.175	37.004	0.952	1.00 48.20	CPS2
ATOM	1489	NE2	GLN	71	83.044	36.069	-0.754	1.00 47.40	CPS2
ATOM	1490	C	GLN	71	82.391	31.578	1.824	1.00 35.81	CPS2
ATOM	1491	O	GLN	71	82.851	31.656	2.962	1.00 36.15	CPS2
ATOM	1492	N	LEU	72	81.257	30.944	1.561	1.00 32.57	CPS2
ATOM	1493	CA	LEU	72	80.461	30.353	2.630	1.00 30.34	CPS2
ATOM	1494	CB	LEU	72	79.503	31.400	3.196	1.00 29.93	CPS2
ATOM	1495	CG	LEU	72	78.560	30.935	4.303	1.00 29.85	CPS2
ATOM	1496	CD1	LEU	72	79.352	30.712	5.585	1.00 29.87	CPS2
ATOM	1497	CD2	LEU	72	77.482	31.998	4.515	1.00 30.13	CPS2
ATOM	1498	C	LEU	72	79.670	29.165	2.117	1.00 28.96	CPS2
ATOM	1499	O	LEU	72	78.925	29.270	1.146	1.00 29.65	CPS2
ATOM	1500	N	SER	73	79.828	28.037	2.791	1.00 26.89	CPS2
ATOM	1501	CA	SER	73	79.163	26.805	2.405	1.00 26.28	CPS2
ATOM	1502	CB	SER	73	80.176	25.656	2.498	1.00 27.70	CPS2
ATOM	1503	OG	SER	73	79.571	24.385	2.324	1.00 31.43	CPS2
ATOM	1504	C	SER	73	77.970	26.491	3.300	1.00 25.59	CPS2
ATOM	1505	O	SER	73	77.912	26.952	4.441	1.00 23.26	CPS2
ATOM	1506	N	PHE	74	77.016	25.718	2.780	1.00 24.61	CPS2
ATOM	1507	CA	PHE	74	75.874	25.292	3.591	1.00 24.32	CPS2
ATOM	1508	CB	PHE	74	74.974	24.333	2.813	1.00 24.91	CPS2
ATOM	1509	CG	PHE	74	74.016	25.012	1.887	1.00 27.32	CPS2
ATOM	1510	CD1	PHE	74	73.041	25.873	2.385	1.00 26.95	CPS2
ATOM	1511	CD2	PHE	74	74.079	24.787	0.511	1.00 28.10	CPS2
ATOM	1512	CE1	PHE	74	72.142	26.501	1.528	1.00 28.03	CPS2
ATOM	1513	CE2	PHE	74	73.185	25.411	-0.350	1.00 29.15	CPS2
ATOM	1514	CZ	PHE	74	72.214	26.271	0.160	1.00 27.71	CPS2
ATOM	1515	C	PHE	74	76.433	24.527	4.788	1.00 25.14	CPS2
ATOM	1516	O	PHE	74	75.841	24.490	5.868	1.00 23.71	CPS2
ATOM	1517	N	GLN	75	77.577	23.886	4.571	1.00 25.35	CPS2
ATOM	1518	CA	GLN	75	78.212	23.099	5.618	1.00 26.61	CPS2
ATOM	1519	CB	GLN	75	79.212	22.115	4.998	1.00 26.65	CPS2
ATOM	1520	CG	GLN	75	78.580	21.089	4.063	1.00 27.20	CPS2
ATOM	1521	CD	GLN	75	77.513	20.259	4.742	1.00 26.33	CPS2
ATOM	1522	OE1	GLN	75	77.695	19.797	5.864	1.00 26.93	CPS2
ATOM	1523	NE2	GLN	75	76.390	20.057	4.056	1.00 27.72	CPS2
ATOM	1524	C	GLN	75	78.918	23.944	6.674	1.00 27.33	CPS2
ATOM	1525	O	GLN	75	79.380	23.413	7.684	1.00 30.23	CPS2
ATOM	1526	N	ASP	76	79.020	25.250	6.455	1.00 28.01	CPS2
ATOM	1527	CA	ASP	76	79.676	26.113	7.441	1.00 26.83	CPS2
ATOM	1528	CB	ASP	76	80.334	27.317	6.769	1.00 28.17	CPS2
ATOM	1529	CG	ASP	76	81.508	26.933	5.900	1.00 29.80	CPS2
ATOM	1530	OD1	ASP	76	82.291	26.066	6.330	1.00 29.26	CPS2
ATOM	1531	OD2	ASP	76	81.649	27.514	4.800	1.00 30.74	CPS2
ATOM	1532	C	ASP	76	78.657	26.648	8.429	1.00 27.59	CPS2
ATOM	1533	O	ASP	76	79.015	27.306	9.412	1.00 26.97	CPS2
ATOM	1534	N	ILE	77	77.389	26.352	8.164	1.00 26.05	CPS2
ATOM	1535	CA	ILE	77	76.280	26.859	8.970	1.00 25.04	CPS2
ATOM	1536	CB	ILE	77	75.306	27.678	8.079	1.00 23.67	CPS2
ATOM	1537	CG2	ILE	77	74.270	28.414	8.942	1.00 24.94	CPS2
ATOM	1538	CG1	ILE	77	76.085	28.674	7.218	1.00 23.77	CPS2

FIG. 1A-27

ATOM	1539	CD1	ILE	77	75.276	29.187	6.019	1.00 23.94	CPS2
ATOM	1540	C	ILE	77	75.487	25.717	9.586	1.00 25.85	CPS2
ATOM	1541	O	ILE	77	75.077	24.796	8.887	1.00 26.62	CPS2
ATOM	1542	N	GLU	78	75.260	25.773	10.892	1.00 24.57	CPS2
ATOM	1543	CA	GLU	78	74.483	24.727	11.529	1.00 24.12	CPS2
ATOM	1544	CB	GLU	78	75.366	23.875	12.450	1.00 24.96	CPS2
ATOM	1545	CG	GLU	78	74.631	22.661	13.039	1.00 26.74	CPS2
ATOM	1546	CD	GLU	78	75.579	21.638	13.643	1.00 30.06	CPS2
ATOM	1547	OE1	GLU	78	75.989	21.815	14.805	1.00 30.41	CPS2
ATOM	1548	OE2	GLU	78	75.930	20.656	12.942	1.00 30.57	CPS2
ATOM	1549	C	GLU	78	73.314	25.285	12.326	1.00 25.19	CPS2
ATOM	1550	O	GLU	78	73.467	26.243	13.096	1.00 24.62	CPS2
ATOM	1551	N	ILE	79	72.139	24.697	12.124	1.00 23.01	CPS2
ATOM	1552	CA	ILE	79	70.969	25.113	12.866	1.00 22.64	CPS2
ATOM	1553	CB	ILE	79	69.673	25.081	12.014	1.00 23.46	CPS2
ATOM	1554	CG2	ILE	79	68.519	25.648	12.832	1.00 25.86	CPS2
ATOM	1555	CG1	ILE	79	69.868	25.835	10.688	1.00 25.21	CPS2
ATOM	1556	CD1	ILE	79	70.337	27.256	10.820	1.00 27.02	CPS2
ATOM	1557	C	ILE	79	70.832	24.078	13.970	1.00 23.01	CPS2
ATOM	1558	O	ILE	79	70.679	22.882	13.691	1.00 22.93	CPS2
ATOM	1559	N	ARG	80	70.912	24.524	15.217	1.00 21.65	CPS2
ATOM	1560	CA	ARG	80	70.765	23.624	16.348	1.00 23.25	CPS2
ATOM	1561	CB	ARG	80	71.928	23.793	17.322	1.00 22.55	CPS2
ATOM	1562	CG	ARG	80	73.275	23.474	16.692	1.00 22.62	CPS2
ATOM	1563	CD	ARG	80	74.373	23.461	17.742	1.00 22.35	CPS2
ATOM	1564	NE	ARG	80	75.680	23.201	17.147	1.00 21.40	CPS2
ATOM	1565	CZ	ARG	80	76.820	23.280	17.823	1.00 22.68	CPS2
ATOM	1566	NH1	ARG	80	76.802	23.614	19.110	1.00 20.04	CPS2
ATOM	1567	NH2	ARG	80	77.971	23.020	17.216	1.00 22.34	CPS2
ATOM	1568	C	ARG	80	69.456	23.947	17.044	1.00 24.16	CPS2
ATOM	1569	O	ARG	80	68.837	24.965	16.757	1.00 23.92	CPS2
ATOM	1570	N	LYS	81	69.028	23.074	17.947	1.00 26.40	CPS2
ATOM	1571	CA	LYS	81	67.789	23.290	18.684	1.00 27.93	CPS2
ATOM	1572	CB	LYS	81	66.840	22.108	18.466	1.00 30.60	CPS2
ATOM	1573	CG	LYS	81	66.517	21.865	17.000	1.00 32.31	CPS2
ATOM	1574	CD	LYS	81	65.759	20.561	16.767	1.00 36.54	CPS2
ATOM	1575	CE	LYS	81	64.326	20.645	17.248	1.00 39.00	CPS2
ATOM	1576	NZ	LYS	81	63.553	19.423	16.848	1.00 41.89	CPS2
ATOM	1577	C	LYS	81	68.113	23.428	20.168	1.00 28.77	CPS2
ATOM	1578	O	LYS	81	68.933	22.671	20.696	1.00 28.58	CPS2
ATOM	1579	N	ASP	82	67.487	24.391	20.837	1.00 27.27	CPS2
ATOM	1580	CA	ASP	82	67.741	24.576	22.258	1.00 29.97	CPS2
ATOM	1581	CB	ASP	82	67.521	26.039	22.666	1.00 28.54	CPS2
ATOM	1582	CG	ASP	82	66.074	26.488	22.541	1.00 30.11	CPS2
ATOM	1583	OD1	ASP	82	65.846	27.715	22.575	1.00 28.52	CPS2
ATOM	1584	OD2	ASP	82	65.170	25.633	22.424	1.00 30.87	CPS2
ATOM	1585	C	ASP	82	66.887	23.619	23.095	1.00 30.91	CPS2
ATOM	1586	O	ASP	82	66.268	22.707	22.546	1.00 30.68	CPS2
ATOM	1587	N	GLN	83	66.867	23.819	24.411	1.00 33.59	CPS2
ATOM	1588	CA	GLN	83	66.120	22.941	25.313	1.00 36.28	CPS2
ATOM	1589	CB	GLN	83	66.334	23.356	26.772	1.00 37.73	CPS2
ATOM	1590	CG	GLN	83	65.575	24.608	27.198	1.00 41.41	CPS2
ATOM	1591	CD	GLN	83	66.435	25.862	27.228	1.00 43.65	CPS2
ATOM	1592	OE1	GLN	83	66.892	26.355	26.187	1.00 44.27	CPS2
ATOM	1593	NE2	GLN	83	66.659	26.389	28.432	1.00 43.27	CPS2
ATOM	1594	C	GLN	83	64.626	22.892	25.022	1.00 37.29	CPS2
ATOM	1595	O	GLN	83	63.943	21.933	25.398	1.00 38.48	CPS2

FIG. 1A-28

ATOM	1596	N	ASN	84	64.120	23.927	24.362	1.00 36.62	CPS2
ATOM	1597	CA	ASN	84	62.707	23.996	24.024	1.00 36.63	CPS2
ATOM	1598	CB	ASN	84	62.168	25.389	24.347	1.00 37.40	CPS2
ATOM	1599	CG	ASN	84	62.263	25.716	25.828	1.00 38.82	CPS2
ATOM	1600	OD1	ASN	84	61.807	24.945	26.675	1.00 39.51	CPS2
ATOM	1601	ND2	ASN	84	62.856	26.857	26.148	1.00 38.34	CPS2
ATOM	1602	C	ASN	84	62.456	23.661	22.556	1.00 36.23	CPS2
ATOM	1603	O	ASN	84	61.345	23.839	22.052	1.00 36.16	CPS2
ATOM	1604	N	GLY	85	63.492	23.173	21.879	1.00 34.68	CPS2
ATOM	1605	CA	GLY	85	63.370	22.814	20.476	1.00 33.60	CPS2
ATOM	1606	C	GLY	85	63.425	23.999	19.523	1.00 32.91	CPS2
ATOM	1607	O	GLY	85	63.210	23.841	18.323	1.00 34.92	CPS2
ATOM	1608	N	LYS	86	63.726	25.184	20.041	1.00 31.20	CPS2
ATOM	1609	CA	LYS	86	63.781	26.379	19.203	1.00 29.67	CPS2
ATOM	1610	CB	LYS	86	63.454	27.605	20.052	1.00 31.80	CPS2
ATOM	1611	CG	LYS	86	62.137	27.394	20.790	1.00 34.73	CPS2
ATOM	1612	CD	LYS	86	61.614	28.628	21.486	1.00 39.19	CPS2
ATOM	1613	CE	LYS	86	60.239	28.331	22.094	1.00 41.01	CPS2
ATOM	1614	NZ	LYS	86	59.558	29.559	22.592	1.00 43.57	CPS2
ATOM	1615	C	LYS	86	65.144	26.492	18.541	1.00 28.23	CPS2
ATOM	1616	O	LYS	86	66.169	26.212	19.159	1.00 27.95	CPS2
ATOM	1617	N	PRO	87	65.173	26.922	17.272	1.00 27.01	CPS2
ATOM	1618	CD	PRO	87	64.035	27.381	16.447	1.00 26.75	CPS2
ATOM	1619	CA	PRO	87	66.427	27.050	16.534	1.00 25.49	CPS2
ATOM	1620	CB	PRO	87	65.951	27.164	15.085	1.00 25.44	CPS2
ATOM	1621	CG	PRO	87	64.735	28.043	15.239	1.00 27.74	CPS2
ATOM	1622	C	PRO	87	67.379	28.185	16.881	1.00 24.72	CPS2
ATOM	1623	O	PRO	87	66.979	29.270	17.306	1.00 23.36	CPS2
ATOM	1624	N	TYR	88	68.664	27.904	16.716	1.00 22.58	CPS2
ATOM	1625	CA	TYR	88	69.685	28.924	16.879	1.00 22.24	CPS2
ATOM	1626	CB	TYR	88	70.208	29.052	18.324	1.00 22.46	CPS2
ATOM	1627	CG	TYR	88	70.921	27.860	18.913	1.00 21.40	CPS2
ATOM	1628	CD1	TYR	88	70.213	26.859	19.577	1.00 21.74	CPS2
ATOM	1629	CE1	TYR	88	70.881	25.796	20.194	1.00 21.69	CPS2
ATOM	1630	CD2	TYR	88	72.317	27.769	18.871	1.00 21.96	CPS2
ATOM	1631	CE2	TYR	88	72.989	26.708	19.480	1.00 20.78	CPS2
ATOM	1632	CZ	TYR	88	72.262	25.731	20.141	1.00 21.27	CPS2
ATOM	1633	OH	TYR	88	72.923	24.699	20.772	1.00 20.50	CPS2
ATOM	1634	C	TYR	88	70.781	28.522	15.912	1.00 22.02	CPS2
ATOM	1635	O	TYR	88	70.897	27.352	15.550	1.00 23.05	CPS2
ATOM	1636	N	ILE	89	71.577	29.485	15.480	1.00 21.04	CPS2
ATOM	1637	CA	ILE	89	72.623	29.198	14.524	1.00 21.06	CPS2
ATOM	1638	CB	ILE	89	72.573	30.209	13.369	1.00 21.84	CPS2
ATOM	1639	CG2	ILE	89	73.842	30.099	12.513	1.00 22.28	CPS2
ATOM	1640	CG1	ILE	89	71.324	29.982	12.522	1.00 22.51	CPS2
ATOM	1641	CD1	ILE	89	71.172	31.035	11.407	1.00 23.39	CPS2
ATOM	1642	C	ILE	89	74.043	29.228	15.072	1.00 22.40	CPS2
ATOM	1643	O	ILE	89	74.401	30.123	15.847	1.00 21.51	CPS2
ATOM	1644	N	ILE	90	74.839	28.248	14.644	1.00 21.66	CPS2
ATOM	1645	CA	ILE	90	76.255	28.184	14.988	1.00 21.61	CPS2
ATOM	1646	CB	ILE	90	76.641	26.878	15.727	1.00 21.37	CPS2
ATOM	1647	CG2	ILE	90	78.169	26.743	15.791	1.00 22.23	CPS2
ATOM	1648	CG1	ILE	90	76.032	26.875	17.134	1.00 20.39	CPS2
ATOM	1649	CD1	ILE	90	76.542	27.991	18.041	1.00 20.47	CPS2
ATOM	1650	C	ILE	90	77.019	28.232	13.664	1.00 22.97	CPS2
ATOM	1651	O	ILE	90	76.763	27.437	12.742	1.00 22.67	CPS2
ATOM	1652	N	CYS	91	77.922	29.195	13.559	1.00 23.95	CPS2

FIG. 1A-29

ATOM	1653	CA	CYS	91	78.769	29.344	12.384	1.00	26.82	CPS2
ATOM	1654	CB	CYS	91	78.229	30.414	11.432	1.00	26.17	CPS2
ATOM	1655	SG	CYS	91	79.260	30.612	9.945	1.00	27.83	CPS2
ATOM	1656	C	CYS	91	80.139	29.760	12.912	1.00	29.07	CPS2
ATOM	1657	O	CYS	91	80.392	30.933	13.149	1.00	29.81	CPS2
ATOM	1658	N	THR	92	81.011	28.784	13.114	1.00	33.43	CPS2
ATOM	1659	CA	THR	92	82.347	29.049	13.637	1.00	37.11	CPS2
ATOM	1660	CB	THR	92	83.080	27.726	13.883	1.00	38.23	CPS2
ATOM	1661	OG1	THR	92	82.422	27.027	14.947	1.00	38.10	CPS2
ATOM	1662	CG2	THR	92	84.536	27.971	14.260	1.00	40.35	CPS2
ATOM	1663	C	THR	92	83.172	29.947	12.719	1.00	39.54	CPS2
ATOM	1664	O	THR	92	84.071	30.663	13.177	1.00	40.49	CPS2
ATOM	1665	N	LYS	93	82.846	29.916	11.432	1.00	40.59	CPS2
ATOM	1666	CA	LYS	93	83.536	30.712	10.428	1.00	44.01	CPS2
ATOM	1667	CB	LYS	93	83.024	30.334	9.040	1.00	45.12	CPS2
ATOM	1668	CG	LYS	93	83.944	30.689	7.889	1.00	47.31	CPS2
ATOM	1669	CD	LYS	93	83.519	29.921	6.650	1.00	47.58	CPS2
ATOM	1670	CE	LYS	93	84.638	29.817	5.630	1.00	48.24	CPS2
ATOM	1671	NZ	LYS	93	84.290	28.834	4.556	1.00	48.73	CPS2
ATOM	1672	C	LYS	93	83.269	32.183	10.690	1.00	44.95	CPS2
ATOM	1673	O	LYS	93	83.901	33.063	10.112	1.00	46.05	CPS2
ATOM	1674	N	LEU	94	82.322	32.443	11.575	1.00	45.51	CPS2
ATOM	1675	CA	LEU	94	81.964	33.803	11.910	1.00	46.37	CPS2
ATOM	1676	CB	LEU	94	80.452	33.898	12.120	1.00	46.46	CPS2
ATOM	1677	CG	LEU	94	79.830	35.271	12.344	1.00	46.35	CPS2
ATOM	1678	CD1	LEU	94	80.037	36.148	11.121	1.00	47.12	CPS2
ATOM	1679	CD2	LEU	94	78.352	35.094	12.615	1.00	46.47	CPS2
ATOM	1680	C	LEU	94	82.685	34.233	13.172	1.00	47.39	CPS2
ATOM	1681	O	LEU	94	82.690	33.511	14.173	1.00	47.30	CPS2
ATOM	1682	N	SER	95	83.319	35.401	13.116	1.00	48.63	CPS2
ATOM	1683	CA	SER	95	84.015	35.941	14.278	1.00	48.81	CPS2
ATOM	1684	CB	SER	95	84.347	37.420	14.037	1.00	49.86	CPS2
ATOM	1685	OG	SER	95	83.229	38.121	13.511	1.00	51.01	CPS2
ATOM	1686	C	SER	95	83.038	35.771	15.448	1.00	48.31	CPS2
ATOM	1687	O	SER	95	81.843	35.585	15.221	1.00	48.26	CPS2
ATOM	1688	N	PRO	96	83.524	35.840	16.704	1.00	46.89	CPS2
ATOM	1689	CD	PRO	96	84.845	36.379	17.068	1.00	46.79	CPS2
ATOM	1690	CA	PRO	96	82.693	35.682	17.909	1.00	45.46	CPS2
ATOM	1691	CB	PRO	96	83.678	35.966	19.040	1.00	45.87	CPS2
ATOM	1692	CG	PRO	96	84.573	36.988	18.434	1.00	45.85	CPS2
ATOM	1693	C	PRO	96	81.431	36.544	18.033	1.00	44.28	CPS2
ATOM	1694	O	PRO	96	81.041	36.911	19.141	1.00	45.08	CPS2
ATOM	1695	N	ALA	97	80.782	36.839	16.913	1.00	41.71	CPS2
ATOM	1696	CA	ALA	97	79.577	37.671	16.900	1.00	38.60	CPS2
ATOM	1697	CB	ALA	97	79.384	38.246	15.507	1.00	39.14	CPS2
ATOM	1698	C	ALA	97	78.288	36.977	17.347	1.00	36.55	CPS2
ATOM	1699	O	ALA	97	78.208	35.752	17.405	1.00	36.57	CPS2
ATOM	1700	N	ALA	98	77.274	37.784	17.651	1.00	33.65	CPS2
ATOM	1701	CA	ALA	98	75.973	37.270	18.065	1.00	30.93	CPS2
ATOM	1702	CB	ALA	98	75.295	38.239	19.026	1.00	29.97	CPS2
ATOM	1703	C	ALA	98	75.125	37.106	16.804	1.00	28.95	CPS2
ATOM	1704	O	ALA	98	75.077	37.990	15.949	1.00	28.62	CPS2
ATOM	1705	N	VAL	99	74.454	35.969	16.709	1.00	26.50	CPS2
ATOM	1706	CA	VAL	99	73.616	35.659	15.566	1.00	23.47	CPS2
ATOM	1707	CB	VAL	99	74.179	34.437	14.806	1.00	23.08	CPS2
ATOM	1708	CG1	VAL	99	73.323	34.125	13.590	1.00	23.46	CPS2
ATOM	1709	CG2	VAL	99	75.617	34.718	14.381	1.00	24.82	CPS2

FIG. 1A-30

ATOM	1710	C	VAL	99	72.209	35.335	16.054	1.00	22.87	CPS2
ATOM	1711	O	VAL	99	72.034	34.549	16.980	1.00	23.69	CPS2
ATOM	1712	N	HIS	100	71.208	35.941	15.430	1.00	21.88	CPS2
ATOM	1713	CA	HIS	100	69.819	35.685	15.800	1.00	20.93	CPS2
ATOM	1714	CB	HIS	100	69.152	36.987	16.248	1.00	22.65	CPS2
ATOM	1715	CG	HIS	100	69.930	37.726	17.296	1.00	24.71	CPS2
ATOM	1716	CD2	HIS	100	70.837	38.727	17.191	1.00	26.85	CPS2
ATOM	1717	ND1	HIS	100	69.841	37.430	18.639	1.00	26.27	CPS2
ATOM	1718	CE1	HIS	100	70.658	38.217	19.318	1.00	28.01	CPS2
ATOM	1719	NE2	HIS	100	71.276	39.012	18.462	1.00	25.52	CPS2
ATOM	1720	C	HIS	100	69.124	35.150	14.553	1.00	19.66	CPS2
ATOM	1721	O	HIS	100	69.414	35.596	13.445	1.00	19.28	CPS2
ATOM	1722	N	VAL	101	68.208	34.203	14.729	1.00	20.06	CPS2
ATOM	1723	CA	VAL	101	67.500	33.628	13.586	1.00	18.60	CPS2
ATOM	1724	CB	VAL	101	68.111	32.251	13.166	1.00	18.24	CPS2
ATOM	1725	CG1	VAL	101	67.973	31.236	14.313	1.00	19.48	CPS2
ATOM	1726	CG2	VAL	101	67.436	31.719	11.884	1.00	16.59	CPS2
ATOM	1727	C	VAL	101	66.053	33.403	13.982	1.00	19.22	CPS2
ATOM	1728	O	VAL	101	65.753	33.247	15.160	1.00	20.38	CPS2
ATOM	1729	N	SER	102	65.155	33.451	13.001	1.00	18.44	CPS2
ATOM	1730	CA	SER	102	63.748	33.140	13.241	1.00	18.74	CPS2
ATOM	1731	CB	SER	102	62.900	34.393	13.455	1.00	18.54	CPS2
ATOM	1732	OG	SER	102	61.588	33.984	13.804	1.00	18.22	CPS2
ATOM	1733	C	SER	102	63.270	32.398	12.006	1.00	18.15	CPS2
ATOM	1734	O	SER	102	63.568	32.801	10.883	1.00	18.21	CPS2
ATOM	1735	N	ILE	103	62.552	31.300	12.207	1.00	18.86	CPS2
ATOM	1736	CA	ILE	103	62.054	30.511	11.079	1.00	18.76	CPS2
ATOM	1737	CB	ILE	103	62.653	29.079	11.109	1.00	19.67	CPS2
ATOM	1738	CG2	ILE	103	62.224	28.298	9.869	1.00	21.39	CPS2
ATOM	1739	CG1	ILE	103	64.184	29.155	11.156	1.00	19.93	CPS2
ATOM	1740	CD1	ILE	103	64.862	27.789	11.269	1.00	21.07	CPS2
ATOM	1741	C	ILE	103	60.537	30.418	11.198	1.00	19.92	CPS2
ATOM	1742	O	ILE	103	60.004	30.291	12.307	1.00	21.12	CPS2
ATOM	1743	N	THR	104	59.840	30.486	10.066	1.00	19.86	CPS2
ATOM	1744	CA	THR	104	58.388	30.396	10.077	1.00	19.62	CPS2
ATOM	1745	CB	THR	104	57.743	31.799	9.944	1.00	21.91	CPS2
ATOM	1746	OG1	THR	104	56.323	31.708	10.159	1.00	22.12	CPS2
ATOM	1747	CG2	THR	104	58.018	32.390	8.573	1.00	20.48	CPS2
ATOM	1748	C	THR	104	57.945	29.487	8.934	1.00	20.91	CPS2
ATOM	1749	O	THR	104	58.722	29.210	8.016	1.00	18.89	CPS2
ATOM	1750	N	HIS	105	56.705	29.015	8.999	1.00	20.52	CPS2
ATOM	1751	CA	HIS	105	56.179	28.108	7.973	1.00	24.14	CPS2
ATOM	1752	CB	HIS	105	56.224	26.647	8.474	1.00	27.48	CPS2
ATOM	1753	CG	HIS	105	57.594	26.134	8.811	1.00	32.26	CPS2
ATOM	1754	CD2	HIS	105	58.267	26.095	9.987	1.00	33.69	CPS2
ATOM	1755	ND1	HIS	105	58.428	25.559	7.874	1.00	34.33	CPS2
ATOM	1756	CE1	HIS	105	59.555	25.191	8.457	1.00	33.58	CPS2
ATOM	1757	NE2	HIS	105	59.484	25.504	9.738	1.00	34.93	CPS2
ATOM	1758	C	HIS	105	54.702	28.393	7.653	1.00	23.87	CPS2
ATOM	1759	O	HIS	105	53.974	28.944	8.476	1.00	23.81	CPS2
ATOM	1760	N	THR	106	54.284	28.013	6.449	1.00	23.91	CPS2
ATOM	1761	CA	THR	106	52.875	28.065	6.054	1.00	24.84	CPS2
ATOM	1762	CB	THR	106	52.484	29.199	5.058	1.00	24.13	CPS2
ATOM	1763	OG1	THR	106	53.116	28.984	3.792	1.00	25.72	CPS2
ATOM	1764	CG2	THR	106	52.841	30.571	5.616	1.00	24.87	CPS2
ATOM	1765	C	THR	106	52.737	26.722	5.339	1.00	26.22	CPS2
ATOM	1766	O	THR	106	53.716	25.971	5.224	1.00	25.93	CPS2

FIG. 1A-31

ATOM	1767	N	LYS	107	51.544	26.408	4.857	1.00	27.42	CPS2
ATOM	1768	CA	LYS	107	51.355	25.135	4.177	1.00	29.72	CPS2
ATOM	1769	CB	LYS	107	49.913	25.013	3.676	1.00	32.60	CPS2
ATOM	1770	CG	LYS	107	49.554	23.612	3.186	1.00	36.45	CPS2
ATOM	1771	CD	LYS	107	48.151	23.568	2.586	1.00	39.60	CPS2
ATOM	1772	CE	LYS	107	48.079	24.346	1.277	1.00	42.78	CPS2
ATOM	1773	NZ	LYS	107	46.750	24.224	0.594	1.00	44.82	CPS2
ATOM	1774	C	LYS	107	52.319	24.941	3.003	1.00	28.95	CPS2
ATOM	1775	O	LYS	107	52.889	23.863	2.833	1.00	29.55	CPS2
ATOM	1776	N	GLU	108	52.524	25.993	2.216	1.00	27.06	CPS2
ATOM	1777	CA	GLU	108	53.374	25.916	1.033	1.00	27.06	CPS2
ATOM	1778	CB	GLU	108	52.639	26.548	-0.155	1.00	29.33	CPS2
ATOM	1779	CG	GLU	108	51.301	25.907	-0.494	1.00	36.04	CPS2
ATOM	1780	CD	GLU	108	51.394	24.407	-0.723	1.00	39.96	CPS2
ATOM	1781	OE1	GLU	108	52.416	23.935	-1.270	1.00	43.61	CPS2
ATOM	1782	OE2	GLU	108	50.430	23.694	-0.370	1.00	43.92	CPS2
ATOM	1783	C	GLU	108	54.771	26.532	1.092	1.00	25.54	CPS2
ATOM	1784	O	GLU	108	55.581	26.311	0.180	1.00	25.56	CPS2
ATOM	1785	N	TYR	109	55.055	27.305	2.138	1.00	24.09	CPS2
ATOM	1786	CA	TYR	109	56.350	27.982	2.250	1.00	21.97	CPS2
ATOM	1787	CB	TYR	109	56.175	29.480	2.012	1.00	23.30	CPS2
ATOM	1788	CG	TYR	109	55.611	29.823	0.664	1.00	24.68	CPS2
ATOM	1789	CD1	TYR	109	56.427	29.842	-0.467	1.00	24.47	CPS2
ATOM	1790	CE1	TYR	109	55.895	30.083	-1.731	1.00	25.63	CPS2
ATOM	1791	CD2	TYR	109	54.248	30.062	0.505	1.00	25.42	CPS2
ATOM	1792	CE2	TYR	109	53.704	30.303	-0.761	1.00	26.80	CPS2
ATOM	1793	CZ	TYR	109	54.530	30.307	-1.866	1.00	25.17	CPS2
ATOM	1794	OH	TYR	109	53.996	30.501	-3.118	1.00	28.15	CPS2
ATOM	1795	C	TYR	109	57.069	27.849	3.578	1.00	21.24	CPS2
ATOM	1796	O	TYR	109	56.465	27.578	4.616	1.00	20.80	CPS2
ATOM	1797	N	ALA	110	58.379	28.067	3.518	1.00	21.00	CPS2
ATOM	1798	CA	ALA	110	59.230	28.102	4.705	1.00	21.72	CPS2
ATOM	1799	CB	ALA	110	60.238	26.966	4.686	1.00	22.11	CPS2
ATOM	1800	C	ALA	110	59.945	29.450	4.560	1.00	21.05	CPS2
ATOM	1801	O	ALA	110	60.301	29.852	3.451	1.00	20.79	CPS2
ATOM	1802	N	ALA	111	60.141	30.165	5.657	1.00	20.04	CPS2
ATOM	1803	CA	ALA	111	60.822	31.446	5.557	1.00	18.91	CPS2
ATOM	1804	CB	ALA	111	59.802	32.577	5.431	1.00	18.42	CPS2
ATOM	1805	C	ALA	111	61.683	31.648	6.785	1.00	17.86	CPS2
ATOM	1806	O	ALA	111	61.400	31.111	7.847	1.00	17.82	CPS2
ATOM	1807	N	ALA	112	62.754	32.411	6.638	1.00	18.38	CPS2
ATOM	1808	CA	ALA	112	63.627	32.642	7.777	1.00	17.98	CPS2
ATOM	1809	CB	ALA	112	64.718	31.564	7.820	1.00	19.37	CPS2
ATOM	1810	C	ALA	112	64.278	33.992	7.650	1.00	18.20	CPS2
ATOM	1811	O	ALA	112	64.414	34.527	6.543	1.00	17.80	CPS2
ATOM	1812	N	GLN	113	64.686	34.540	8.787	1.00	16.99	CPS2
ATOM	1813	CA	GLN	113	65.406	35.802	8.775	1.00	19.02	CPS2
ATOM	1814	CB	GLN	113	64.511	36.964	9.178	1.00	21.92	CPS2
ATOM	1815	CG	GLN	113	64.045	36.908	10.593	1.00	24.71	CPS2
ATOM	1816	CD	GLN	113	63.223	38.120	10.979	1.00	27.15	CPS2
ATOM	1817	OE1	GLN	113	62.785	38.239	12.117	1.00	29.66	CPS2
ATOM	1818	NE2	GLN	113	63.001	39.019	10.028	1.00	31.94	CPS2
ATOM	1819	C	GLN	113	66.554	35.662	9.764	1.00	18.49	CPS2
ATOM	1820	O	GLN	113	66.463	34.908	10.738	1.00	18.27	CPS2
ATOM	1821	N	VAL	114	67.626	36.395	9.506	1.00	18.07	CPS2
ATOM	1822	CA	VAL	114	68.811	36.355	10.358	1.00	18.90	CPS2
ATOM	1823	CB	VAL	114	69.939	35.488	9.698	1.00	19.24	CPS2

FIG. 1A-32

ATOM	1824	CG1	VAL	114	71.288	35.715	10.406	1.00	20.55	CPS2
ATOM	1825	CG2	VAL	114	69.575	34.007	9.753	1.00	20.65	CPS2
ATOM	1826	C	VAL	114	69.369	37.757	10.551	1.00	18.95	CPS2
ATOM	1827	O	VAL	114	69.283	38.595	9.653	1.00	18.70	CPS2
ATOM	1828	N	VAL	115	69.918	38.015	11.733	1.00	18.92	CPS2
ATOM	1829	CA	VAL	115	70.580	39.291	11.989	1.00	19.34	CPS2
ATOM	1830	CB	VAL	115	69.805	40.208	12.970	1.00	19.17	CPS2
ATOM	1831	CG1	VAL	115	70.668	41.445	13.298	1.00	20.91	CPS2
ATOM	1832	CG2	VAL	115	68.499	40.688	12.334	1.00	18.48	CPS2
ATOM	1833	C	VAL	115	71.915	38.927	12.633	1.00	21.35	CPS2
ATOM	1834	O	VAL	115	71.949	38.164	13.590	1.00	21.11	CPS2
ATOM	1835	N	ILE	116	73.009	39.428	12.074	1.00	22.97	CPS2
ATOM	1836	CA	ILE	116	74.333	39.174	12.641	1.00	25.35	CPS2
ATOM	1837	CB	ILE	116	75.359	38.779	11.554	1.00	24.57	CPS2
ATOM	1838	CG2	ILE	116	76.752	38.641	12.177	1.00	25.34	CPS2
ATOM	1839	CG1	ILE	116	74.945	37.468	10.880	1.00	23.64	CPS2
ATOM	1840	CD1	ILE	116	75.862	37.065	9.734	1.00	24.45	CPS2
ATOM	1841	C	ILE	116	74.763	40.511	13.243	1.00	27.82	CPS2
ATOM	1842	O	ILE	116	74.692	41.531	12.569	1.00	26.14	CPS2
ATOM	1843	N	GLU	117	75.176	40.508	14.508	1.00	31.83	CPS2
ATOM	1844	CA	GLU	117	75.620	41.741	15.162	1.00	38.95	CPS2
ATOM	1845	CB	GLU	117	75.075	41.848	16.583	1.00	40.48	CPS2
ATOM	1846	CG	GLU	117	73.585	41.670	16.763	1.00	42.57	CPS2
ATOM	1847	CD	GLU	117	73.180	41.900	18.211	1.00	43.48	CPS2
ATOM	1848	OE1	GLU	117	73.040	43.075	18.613	1.00	45.02	CPS2
ATOM	1849	OE2	GLU	117	73.029	40.909	18.956	1.00	43.86	CPS2
ATOM	1850	C	GLU	117	77.140	41.701	15.260	1.00	42.69	CPS2
ATOM	1851	O	GLU	117	77.707	40.665	15.598	1.00	44.02	CPS2
ATOM	1852	N	ARG	118	77.803	42.820	14.989	1.00	46.91	CPS2
ATOM	1853	CA	ARG	118	79.259	42.843	15.069	1.00	50.26	CPS2
ATOM	1854	CB	ARG	118	79.824	43.901	14.124	1.00	52.17	CPS2
ATOM	1855	CG	ARG	118	79.547	45.337	14.529	1.00	54.69	CPS2
ATOM	1856	CD	ARG	118	79.478	46.208	13.288	1.00	57.22	CPS2
ATOM	1857	NE	ARG	118	80.501	45.827	12.319	1.00	59.20	CPS2
ATOM	1858	CZ	ARG	118	80.479	46.170	11.034	1.00	60.31	CPS2
ATOM	1859	NH1	ARG	118	79.483	46.906	10.556	1.00	60.38	CPS2
ATOM	1860	NH2	ARG	118	81.451	45.769	10.224	1.00	60.45	CPS2
ATOM	1861	C	ARG	118	79.722	43.108	16.499	1.00	51.12	CPS2
ATOM	1862	OT1	ARG	118	78.849	43.285	17.380	1.00	51.54	CPS2
ATOM	1863	OT2	ARG	118	80.952	43.125	16.721	1.00	52.39	CPS2
ATOM	1864	C	GLY	1	70.826	44.611	21.183	1.00	31.20	CPS3
ATOM	1865	O	GLY	1	69.832	44.954	21.818	1.00	30.54	CPS3
ATOM	1866	N	GLY	1	72.197	46.046	22.695	1.00	34.55	CPS3
ATOM	1867	CA	GLY	1	72.168	45.285	21.411	1.00	32.26	CPS3
ATOM	1868	N	ILE	2	70.797	43.643	20.274	1.00	29.14	CPS3
ATOM	1869	CA	ILE	2	69.562	42.935	19.973	1.00	27.23	CPS3
ATOM	1870	CB	ILE	2	69.544	42.452	18.510	1.00	28.42	CPS3
ATOM	1871	CG2	ILE	2	68.334	41.538	18.271	1.00	29.40	CPS3
ATOM	1872	CG1	ILE	2	69.495	43.670	17.576	1.00	28.86	CPS3
ATOM	1873	CD1	ILE	2	69.507	43.331	16.115	1.00	31.24	CPS3
ATOM	1874	C	ILE	2	69.332	41.748	20.883	1.00	26.26	CPS3
ATOM	1875	O	ILE	2	70.213	40.893	21.040	1.00	25.80	CPS3
ATOM	1876	N	TYR	3	68.147	41.713	21.489	1.00	24.05	CPS3
ATOM	1877	CA	TYR	3	67.752	40.622	22.369	1.00	24.41	CPS3
ATOM	1878	CB	TYR	3	66.682	41.080	23.352	1.00	26.14	CPS3
ATOM	1879	CG	TYR	3	66.254	39.967	24.268	1.00	28.89	CPS3
ATOM	1880	CD1	TYR	3	67.098	39.514	25.290	1.00	29.65	CPS3

FIG. 1A-33

ATOM	1881	CE1	TYR	3	66.736	38.442	26.092	1.00	32.21	CPS3
ATOM	1882	CD2	TYR	3	65.037	39.316	24.080	1.00	29.35	CPS3
ATOM	1883	CE2	TYR	3	64.667	38.235	24.883	1.00	31.35	CPS3
ATOM	1884	CZ	TYR	3	65.520	37.806	25.881	1.00	32.89	CPS3
ATOM	1885	OH	TYR	3	65.160	36.730	26.660	1.00	35.01	CPS3
ATOM	1886	C	TYR	3	67.190	39.454	21.551	1.00	23.32	CPS3
ATOM	1887	O	TYR	3	67.604	38.305	21.720	1.00	22.34	CPS3
ATOM	1888	N	GLY	4	66.240	39.755	20.667	1.00	21.28	CPS3
ATOM	1889	CA	GLY	4	65.655	38.705	19.848	1.00	20.37	CPS3
ATOM	1890	C	GLY	4	64.945	39.231	18.614	1.00	18.42	CPS3
ATOM	1891	O	GLY	4	64.636	40.411	18.527	1.00	18.04	CPS3
ATOM	1892	N	ILE	5	64.694	38.350	17.656	1.00	17.82	CPS3
ATOM	1893	CA	ILE	5	63.990	38.736	16.432	1.00	17.02	CPS3
ATOM	1894	CB	ILE	5	64.939	38.802	15.206	1.00	16.53	CPS3
ATOM	1895	CG2	ILE	5	66.110	39.753	15.514	1.00	17.11	CPS3
ATOM	1896	CG1	ILE	5	65.457	37.398	14.841	1.00	16.93	CPS3
ATOM	1897	CD1	ILE	5	66.404	37.390	13.622	1.00	18.91	CPS3
ATOM	1898	C	ILE	5	62.932	37.669	16.202	1.00	17.16	CPS3
ATOM	1899	O	ILE	5	63.033	36.555	16.737	1.00	16.49	CPS3
ATOM	1900	N	GLY	6	61.900	38.010	15.441	1.00	16.65	CPS3
ATOM	1901	CA	GLY	6	60.847	37.041	15.187	1.00	17.04	CPS3
ATOM	1902	C	GLY	6	60.217	37.338	13.844	1.00	17.86	CPS3
ATOM	1903	O	GLY	6	60.070	38.500	13.472	1.00	16.46	CPS3
ATOM	1904	N	LEU	7	59.865	36.283	13.110	1.00	18.17	CPS3
ATOM	1905	CA	LEU	7	59.257	36.432	11.795	1.00	18.15	CPS3
ATOM	1906	CB	LEU	7	60.258	36.047	10.698	1.00	17.40	CPS3
ATOM	1907	CG	LEU	7	59.723	35.991	9.257	1.00	17.71	CPS3
ATOM	1908	CD1	LEU	7	59.370	37.420	8.785	1.00	18.00	CPS3
ATOM	1909	CD2	LEU	7	60.775	35.357	8.330	1.00	18.26	CPS3
ATOM	1910	C	LEU	7	58.068	35.482	11.718	1.00	18.31	CPS3
ATOM	1911	O	LEU	7	58.121	34.371	12.236	1.00	18.61	CPS3
ATOM	1912	N	ASP	8	56.992	35.923	11.083	1.00	18.46	CPS3
ATOM	1913	CA	ASP	8	55.849	35.043	10.911	1.00	18.86	CPS3
ATOM	1914	CB	ASP	8	54.871	35.157	12.082	1.00	19.63	CPS3
ATOM	1915	CG	ASP	8	53.642	34.294	11.881	1.00	22.43	CPS3
ATOM	1916	OD1	ASP	8	52.653	34.768	11.281	1.00	23.32	CPS3
ATOM	1917	OD2	ASP	8	53.683	33.126	12.294	1.00	24.61	CPS3
ATOM	1918	C	ASP	8	55.107	35.350	9.632	1.00	19.01	CPS3
ATOM	1919	O	ASP	8	54.955	36.507	9.251	1.00	19.92	CPS3
ATOM	1920	N	ILE	9	54.671	34.302	8.946	1.00	18.64	CPS3
ATOM	1921	CA	ILE	9	53.871	34.490	7.747	1.00	20.14	CPS3
ATOM	1922	CB	ILE	9	54.565	33.982	6.468	1.00	19.98	CPS3
ATOM	1923	CG2	ILE	9	53.605	34.144	5.283	1.00	20.49	CPS3
ATOM	1924	CG1	ILE	9	55.843	34.782	6.213	1.00	20.86	CPS3
ATOM	1925	CD1	ILE	9	56.635	34.318	4.987	1.00	23.49	CPS3
ATOM	1926	C	ILE	9	52.642	33.649	8.032	1.00	20.08	CPS3
ATOM	1927	O	ILE	9	52.760	32.500	8.472	1.00	21.18	CPS3
ATOM	1928	N	THR	10	51.470	34.224	7.793	1.00	20.82	CPS3
ATOM	1929	CA	THR	10	50.218	33.543	8.064	1.00	22.22	CPS3
ATOM	1930	CB	THR	10	49.502	34.213	9.267	1.00	23.80	CPS3
ATOM	1931	OG1	THR	10	50.237	33.942	10.478	1.00	22.74	CPS3
ATOM	1932	CG2	THR	10	48.088	33.667	9.413	1.00	24.86	CPS3
ATOM	1933	C	THR	10	49.310	33.548	6.838	1.00	22.47	CPS3
ATOM	1934	O	THR	10	49.106	34.581	6.197	1.00	22.06	CPS3
ATOM	1935	N	GLU	11	48.784	32.377	6.508	1.00	23.62	CPS3
ATOM	1936	CA	GLU	11	47.894	32.230	5.359	1.00	25.07	CPS3
ATOM	1937	CB	GLU	11	47.846	30.757	4.940	1.00	25.66	CPS3

FIG. 1A-34

ATOM	1938	CG	GLU	11	46.898	30.463	3.793	1.00	29.78	CPS3
ATOM	1939	CD	GLU	11	46.798	28.980	3.481	1.00	32.43	CPS3
ATOM	1940	OE1	GLU	11	47.101	28.151	4.373	1.00	34.21	CPS3
ATOM	1941	OE2	GLU	11	46.396	28.643	2.346	1.00	34.51	CPS3
ATOM	1942	C	GLU	11	46.502	32.708	5.771	1.00	25.06	CPS3
ATOM	1943	O	GLU	11	45.922	32.173	6.714	1.00	25.54	CPS3
ATOM	1944	N	LEU	12	45.963	33.701	5.069	1.00	25.35	CPS3
ATOM	1945	CA	LEU	12	44.642	34.234	5.403	1.00	26.43	CPS3
ATOM	1946	CB	LEU	12	44.225	35.329	4.408	1.00	28.34	CPS3
ATOM	1947	CG	LEU	12	44.432	36.787	4.846	1.00	30.12	CPS3
ATOM	1948	CD1	LEU	12	45.896	37.051	5.095	1.00	29.84	CPS3
ATOM	1949	CD2	LEU	12	43.898	37.731	3.771	1.00	31.67	CPS3
ATOM	1950	C	LEU	12	43.552	33.163	5.459	1.00	27.18	CPS3
ATOM	1951	O	LEU	12	42.700	33.183	6.350	1.00	25.07	CPS3
ATOM	1952	N	ALA	13	43.585	32.231	4.511	1.00	26.60	CPS3
ATOM	1953	CA	ALA	13	42.602	31.160	4.467	1.00	27.39	CPS3
ATOM	1954	CB	ALA	13	42.836	30.296	3.227	1.00	28.53	CPS3
ATOM	1955	C	ALA	13	42.616	30.293	5.730	1.00	28.85	CPS3
ATOM	1956	O	ALA	13	41.569	29.793	6.158	1.00	29.11	CPS3
ATOM	1957	N	ARG	14	43.790	30.115	6.332	1.00	28.68	CPS3
ATOM	1958	CA	ARG	14	43.898	29.303	7.536	1.00	29.64	CPS3
ATOM	1959	CB	ARG	14	45.361	28.961	7.844	1.00	31.16	CPS3
ATOM	1960	CG	ARG	14	45.520	27.811	8.831	1.00	33.62	CPS3
ATOM	1961	CD	ARG	14	46.961	27.333	8.931	1.00	36.46	CPS3
ATOM	1962	NE	ARG	14	47.813	28.263	9.669	1.00	39.10	CPS3
ATOM	1963	CZ	ARG	14	47.809	28.400	10.993	1.00	39.42	CPS3
ATOM	1964	NH1	ARG	14	46.998	27.665	11.741	1.00	41.04	CPS3
ATOM	1965	NH2	ARG	14	48.618	29.273	11.572	1.00	39.96	CPS3
ATOM	1966	C	ARG	14	43.277	30.067	8.693	1.00	30.10	CPS3
ATOM	1967	O	ARG	14	42.619	29.473	9.549	1.00	30.68	CPS3
ATOM	1968	N	ILE	15	43.490	31.382	8.721	1.00	28.50	CPS3
ATOM	1969	CA	ILE	15	42.904	32.220	9.765	1.00	29.44	CPS3
ATOM	1970	CB	ILE	15	43.322	33.708	9.611	1.00	28.52	CPS3
ATOM	1971	CG2	ILE	15	42.492	34.596	10.544	1.00	27.32	CPS3
ATOM	1972	CG1	ILE	15	44.809	33.865	9.955	1.00	27.87	CPS3
ATOM	1973	CD1	ILE	15	45.145	33.454	11.384	1.00	29.13	CPS3
ATOM	1974	C	ILE	15	41.383	32.116	9.656	1.00	30.89	CPS3
ATOM	1975	O	ILE	15	40.689	31.904	10.654	1.00	31.81	CPS3
ATOM	1976	N	ALA	16	40.868	32.271	8.439	1.00	31.30	CPS3
ATOM	1977	CA	ALA	16	39.427	32.180	8.223	1.00	33.08	CPS3
ATOM	1978	CB	ALA	16	39.096	32.463	6.760	1.00	33.09	CPS3
ATOM	1979	C	ALA	16	38.902	30.802	8.634	1.00	34.30	CPS3
ATOM	1980	O	ALA	16	37.800	30.695	9.169	1.00	35.45	CPS3
ATOM	1981	N	SER	17	39.689	29.753	8.395	1.00	35.66	CPS3
ATOM	1982	CA	SER	17	39.282	28.396	8.764	1.00	38.32	CPS3
ATOM	1983	CB	SER	17	40.271	27.356	8.227	1.00	39.07	CPS3
ATOM	1984	OG	SER	17	40.290	27.332	6.810	1.00	40.78	CPS3
ATOM	1985	C	SER	17	39.187	28.242	10.277	1.00	40.41	CPS3
ATOM	1986	O	SER	17	38.202	27.704	10.789	1.00	40.87	CPS3
ATOM	1987	N	MET	18	40.215	28.704	10.989	1.00	41.04	CPS3
ATOM	1988	CA	MET	18	40.238	28.621	12.449	1.00	42.44	CPS3
ATOM	1989	CB	MET	18	41.582	29.110	13.004	1.00	42.96	CPS3
ATOM	1990	CG	MET	18	42.774	28.251	12.617	1.00	44.33	CPS3
ATOM	1991	SD	MET	18	44.266	28.670	13.558	1.00	48.01	CPS3
ATOM	1992	CE	MET	18	44.718	30.192	12.791	1.00	43.96	CPS3
ATOM	1993	C	MET	18	39.115	29.448	13.055	1.00	42.50	CPS3
ATOM	1994	O	MET	18	38.472	29.026	14.014	1.00	43.21	CPS3

FIG. 1A-35

ATOM	1995	N	ALA	19	38.886	30.629	12.496	1.00	43.10	CPS3
ATOM	1996	CA	ALA	19	37.838	31.517	12.981	1.00	44.50	CPS3
ATOM	1997	CB	ALA	19	37.901	32.844	12.233	1.00	45.06	CPS3
ATOM	1998	C	ALA	19	36.453	30.889	12.816	1.00	46.48	CPS3
ATOM	1999	O	ALA	19	35.541	31.155	13.603	1.00	46.54	CPS3
ATOM	2000	N	GLY	20	36.296	30.061	11.788	1.00	47.19	CPS3
ATOM	2001	CA	GLY	20	35.015	29.417	11.558	1.00	48.52	CPS3
ATOM	2002	C	GLY	20	34.838	28.190	12.429	1.00	48.97	CPS3
ATOM	2003	O	GLY	20	33.754	27.928	12.945	1.00	49.64	CPS3
ATOM	2004	N	ARG	21	35.921	27.443	12.599	1.00	49.96	CPS3
ATOM	2005	CA	ARG	21	35.915	26.227	13.397	1.00	50.93	CPS3
ATOM	2006	CB	ARG	21	37.083	25.336	12.963	1.00	52.93	CPS3
ATOM	2007	CG	ARG	21	37.367	24.152	13.872	1.00	55.96	CPS3
ATOM	2008	CD	ARG	21	36.136	23.278	14.055	1.00	58.49	CPS3
ATOM	2009	NE	ARG	21	36.396	22.145	14.940	1.00	60.33	CPS3
ATOM	2010	CZ	ARG	21	35.448	21.371	15.457	1.00	60.98	CPS3
ATOM	2011	NH1	ARG	21	34.171	21.611	15.179	1.00	61.06	CPS3
ATOM	2012	NH2	ARG	21	35.776	20.356	16.247	1.00	61.52	CPS3
ATOM	2013	C	ARG	21	35.987	26.469	14.904	1.00	51.00	CPS3
ATOM	2014	O	ARG	21	35.437	25.698	15.693	1.00	51.31	CPS3
ATOM	2015	N	GLN	22	36.655	27.543	15.307	1.00	50.09	CPS3
ATOM	2016	CA	GLN	22	36.807	27.835	16.725	1.00	49.10	CPS3
ATOM	2017	CB	GLN	22	38.224	28.330	17.011	1.00	48.88	CPS3
ATOM	2018	CG	GLN	22	39.273	27.241	16.967	1.00	49.46	CPS3
ATOM	2019	CD	GLN	22	40.653	27.759	17.297	1.00	49.87	CPS3
ATOM	2020	OE1	GLN	22	40.828	28.529	18.242	1.00	50.04	CPS3
ATOM	2021	NE2	GLN	22	41.648	27.330	16.526	1.00	50.52	CPS3
ATOM	2022	C	GLN	22	35.822	28.816	17.328	1.00	47.67	CPS3
ATOM	2023	O	GLN	22	35.309	29.716	16.660	1.00	48.35	CPS3
ATOM	2024	N	LYS	23	35.580	28.626	18.619	1.00	46.19	CPS3
ATOM	2025	CA	LYS	23	34.683	29.477	19.384	1.00	44.06	CPS3
ATOM	2026	CB	LYS	23	34.086	28.701	20.569	1.00	45.41	CPS3
ATOM	2027	CG	LYS	23	34.474	27.218	20.651	1.00	48.30	CPS3
ATOM	2028	CD	LYS	23	35.983	27.019	20.828	1.00	50.15	CPS3
ATOM	2029	CE	LYS	23	36.341	25.554	21.037	1.00	51.50	CPS3
ATOM	2030	NZ	LYS	23	35.720	25.007	22.285	1.00	51.24	CPS3
ATOM	2031	C	LYS	23	35.490	30.659	19.918	1.00	40.79	CPS3
ATOM	2032	O	LYS	23	36.523	30.457	20.558	1.00	40.61	CPS3
ATOM	2033	N	ARG	24	35.029	31.878	19.630	1.00	36.53	CPS3
ATOM	2034	CA	ARG	24	35.671	33.110	20.103	1.00	33.31	CPS3
ATOM	2035	CB	ARG	24	35.675	33.153	21.630	1.00	32.78	CPS3
ATOM	2036	CG	ARG	24	34.367	32.793	22.310	1.00	34.25	CPS3
ATOM	2037	CD	ARG	24	33.299	33.846	22.126	1.00	35.40	CPS3
ATOM	2038	NE	ARG	24	32.105	33.476	22.883	1.00	38.23	CPS3
ATOM	2039	CZ	ARG	24	30.866	33.783	22.520	1.00	38.00	CPS3
ATOM	2040	NH1	ARG	24	30.653	34.474	21.405	1.00	38.06	CPS3
ATOM	2041	NH2	ARG	24	29.841	33.375	23.259	1.00	39.67	CPS3
ATOM	2042	C	ARG	24	37.116	33.301	19.641	1.00	31.71	CPS3
ATOM	2043	O	ARG	24	37.930	33.845	20.393	1.00	27.62	CPS3
ATOM	2044	N	PHE	25	37.441	32.880	18.421	1.00	29.27	CPS3
ATOM	2045	CA	PHE	25	38.816	33.016	17.950	1.00	28.40	CPS3
ATOM	2046	CB	PHE	25	38.958	32.446	16.539	1.00	28.43	CPS3
ATOM	2047	CG	PHE	25	40.370	32.482	16.011	1.00	28.82	CPS3
ATOM	2048	CD1	PHE	25	40.758	33.450	15.097	1.00	29.33	CPS3
ATOM	2049	CD2	PHE	25	41.311	31.556	16.445	1.00	30.13	CPS3
ATOM	2050	CE1	PHE	25	42.067	33.500	14.618	1.00	30.52	CPS3
ATOM	2051	CE2	PHE	25	42.625	31.597	15.970	1.00	30.21	CPS3

FIG. 1A-36

ATOM	2052	CZ	PHE	25	42.997	32.570	15.059	1.00	29.47	CPS3
ATOM	2053	C	PHE	25	39.325	34.455	17.992	1.00	27.06	CPS3
ATOM	2054	O	PHE	25	40.394	34.716	18.531	1.00	27.13	CPS3
ATOM	2055	N	ALA	26	38.569	35.394	17.433	1.00	27.40	CPS3
ATOM	2056	CA	ALA	26	38.996	36.793	17.441	1.00	26.90	CPS3
ATOM	2057	CB	ALA	26	37.987	37.661	16.692	1.00	27.98	CPS3
ATOM	2058	C	ALA	26	39.174	37.302	18.869	1.00	26.90	CPS3
ATOM	2059	O	ALA	26	40.131	38.027	19.170	1.00	25.61	CPS3
ATOM	2060	N	GLU	27	38.254	36.912	19.753	1.00	25.63	CPS3
ATOM	2061	CA	GLU	27	38.314	37.329	21.143	1.00	25.29	CPS3
ATOM	2062	CB	GLU	27	37.070	36.864	21.908	1.00	25.87	CPS3
ATOM	2063	CG	GLU	27	35.815	37.656	21.612	1.00	26.46	CPS3
ATOM	2064	CD	GLU	27	35.199	37.336	20.266	1.00	28.64	CPS3
ATOM	2065	OE1	GLU	27	35.569	36.324	19.633	1.00	29.62	CPS3
ATOM	2066	OE2	GLU	27	34.319	38.106	19.845	1.00	31.82	CPS3
ATOM	2067	C	GLU	27	39.548	36.770	21.835	1.00	24.48	CPS3
ATOM	2068	O	GLU	27	40.026	37.340	22.812	1.00	23.69	CPS3
ATOM	2069	N	ARG	28	40.057	35.652	21.336	1.00	24.10	CPS3
ATOM	2070	CA	ARG	28	41.235	35.046	21.937	1.00	25.35	CPS3
ATOM	2071	CB	ARG	28	41.286	33.561	21.588	1.00	26.74	CPS3
ATOM	2072	CG	ARG	28	42.365	32.796	22.331	1.00	30.57	CPS3
ATOM	2073	CD	ARG	28	42.064	31.303	22.339	1.00	33.01	CPS3
ATOM	2074	NE	ARG	28	42.094	30.724	21.001	1.00	34.13	CPS3
ATOM	2075	CZ	ARG	28	43.212	30.481	20.327	1.00	36.89	CPS3
ATOM	2076	NH1	ARG	28	44.389	30.768	20.871	1.00	37.04	CPS3
ATOM	2077	NH2	ARG	28	43.157	29.946	19.111	1.00	37.15	CPS3
ATOM	2078	C	ARG	28	42.529	35.736	21.488	1.00	24.56	CPS3
ATOM	2079	O	ARG	28	43.450	35.930	22.282	1.00	24.22	CPS3
ATOM	2080	N	ILE	29	42.574	36.130	20.225	1.00	23.52	CPS3
ATOM	2081	CA	ILE	29	43.760	36.773	19.657	1.00	24.20	CPS3
ATOM	2082	CB	ILE	29	43.788	36.591	18.122	1.00	24.82	CPS3
ATOM	2083	CG2	ILE	29	45.074	37.184	17.538	1.00	25.66	CPS3
ATOM	2084	CG1	ILE	29	43.627	35.107	17.768	1.00	26.45	CPS3
ATOM	2085	CD1	ILE	29	44.675	34.207	18.357	1.00	26.17	CPS3
ATOM	2086	C	ILE	29	43.866	38.270	19.932	1.00	24.20	CPS3
ATOM	2087	O	ILE	29	44.964	38.795	20.164	1.00	23.59	CPS3
ATOM	2088	N	LEU	30	42.722	38.952	19.913	1.00	22.23	CPS3
ATOM	2089	CA	LEU	30	42.683	40.401	20.076	1.00	22.20	CPS3
ATOM	2090	CB	LEU	30	41.643	40.977	19.106	1.00	21.52	CPS3
ATOM	2091	CG	LEU	30	41.738	40.518	17.649	1.00	22.01	CPS3
ATOM	2092	CD1	LEU	30	40.591	41.151	16.857	1.00	22.54	CPS3
ATOM	2093	CD2	LEU	30	43.104	40.926	17.051	1.00	22.99	CPS3
ATOM	2094	C	LEU	30	42.387	40.940	21.467	1.00	22.82	CPS3
ATOM	2095	O	LEU	30	41.622	40.342	22.216	1.00	22.70	CPS3
ATOM	2096	N	THR	31	42.995	42.080	21.798	1.00	22.58	CPS3
ATOM	2097	CA	THR	31	42.752	42.741	23.076	1.00	23.08	CPS3
ATOM	2098	CB	THR	31	43.781	43.846	23.374	1.00	22.96	CPS3
ATOM	2099	OG1	THR	31	43.666	44.871	22.377	1.00	23.51	CPS3
ATOM	2100	CG2	THR	31	45.200	43.283	23.406	1.00	23.16	CPS3
ATOM	2101	C	THR	31	41.400	43.438	22.944	1.00	23.05	CPS3
ATOM	2102	O	THR	31	40.840	43.499	21.850	1.00	20.90	CPS3
ATOM	2103	N	ARG	32	40.887	43.992	24.042	1.00	23.64	CPS3
ATOM	2104	CA	ARG	32	39.593	44.672	23.984	1.00	25.29	CPS3
ATOM	2105	CB	ARG	32	39.224	45.258	25.346	1.00	24.83	CPS3
ATOM	2106	CG	ARG	32	39.005	44.220	26.419	1.00	26.80	CPS3
ATOM	2107	CD	ARG	32	38.684	44.890	27.752	1.00	25.11	CPS3
ATOM	2108	NE	ARG	32	38.513	43.908	28.819	1.00	25.70	CPS3

FIG. 1A-37

ATOM	2109	CZ	ARG	32	38.361	44.218	30.101	1.00	25.97	CPS3
ATOM	2110	NH1	ARG	32	38.357	45.492	30.481	1.00	26.33	CPS3
ATOM	2111	NH2	ARG	32	38.224	43.256	31.005	1.00	27.07	CPS3
ATOM	2112	C	ARG	32	39.570	45.789	22.953	1.00	25.39	CPS3
ATOM	2113	O	ARG	32	38.608	45.912	22.187	1.00	24.58	CPS3
ATOM	2114	N	SER	33	40.622	46.605	22.935	1.00	24.96	CPS3
ATOM	2115	CA	SER	33	40.699	47.715	21.988	1.00	25.69	CPS3
ATOM	2116	CB	SER	33	41.909	48.603	22.284	1.00	27.21	CPS3
ATOM	2117	OG	SER	33	41.714	49.345	23.469	1.00	28.30	CPS3
ATOM	2118	C	SER	33	40.766	47.250	20.544	1.00	25.41	CPS3
ATOM	2119	O	SER	33	40.180	47.870	19.664	1.00	25.68	CPS3
ATOM	2120	N	GLU	34	41.492	46.169	20.290	1.00	24.03	CPS3
ATOM	2121	CA	GLU	34	41.597	45.640	18.935	1.00	23.95	CPS3
ATOM	2122	CB	GLU	34	42.699	44.574	18.879	1.00	23.46	CPS3
ATOM	2123	CG	GLU	34	44.089	45.163	19.059	1.00	21.69	CPS3
ATOM	2124	CD	GLU	34	45.182	44.105	19.221	1.00	22.84	CPS3
ATOM	2125	OE1	GLU	34	46.328	44.405	18.837	1.00	21.34	CPS3
ATOM	2126	OE2	GLU	34	44.900	42.996	19.740	1.00	20.06	CPS3
ATOM	2127	C	GLU	34	40.244	45.051	18.516	1.00	25.26	CPS3
ATOM	2128	O	GLU	34	39.846	45.151	17.353	1.00	25.38	CPS3
ATOM	2129	N	LEU	35	39.548	44.433	19.472	1.00	24.79	CPS3
ATOM	2130	CA	LEU	35	38.231	43.849	19.211	1.00	25.97	CPS3
ATOM	2131	CB	LEU	35	37.678	43.160	20.462	1.00	27.07	CPS3
ATOM	2132	CG	LEU	35	37.717	41.639	20.630	1.00	30.32	CPS3
ATOM	2133	CD1	LEU	35	36.834	41.312	21.844	1.00	30.54	CPS3
ATOM	2134	CD2	LEU	35	37.201	40.893	19.391	1.00	28.41	CPS3
ATOM	2135	C	LEU	35	37.264	44.947	18.806	1.00	25.13	CPS3
ATOM	2136	O	LEU	35	36.471	44.778	17.885	1.00	26.21	CPS3
ATOM	2137	N	ASP	36	37.310	46.066	19.518	1.00	25.47	CPS3
ATOM	2138	CA	ASP	36	36.432	47.180	19.189	1.00	26.39	CPS3
ATOM	2139	CB	ASP	36	36.696	48.383	20.111	1.00	27.06	CPS3
ATOM	2140	CG	ASP	36	36.203	48.148	21.531	1.00	30.18	CPS3
ATOM	2141	OD1	ASP	36	35.336	47.272	21.710	1.00	28.81	CPS3
ATOM	2142	OD2	ASP	36	36.667	48.843	22.464	1.00	29.67	CPS3
ATOM	2143	C	ASP	36	36.638	47.580	17.733	1.00	28.21	CPS3
ATOM	2144	O	ASP	36	35.674	47.866	17.024	1.00	27.00	CPS3
ATOM	2145	N	GLN	37	37.892	47.580	17.281	1.00	28.66	CPS3
ATOM	2146	CA	GLN	37	38.200	47.939	15.895	1.00	28.46	CPS3
ATOM	2147	CB	GLN	37	39.712	48.129	15.705	1.00	31.40	CPS3
ATOM	2148	CG	GLN	37	40.309	49.384	16.315	1.00	34.73	CPS3
ATOM	2149	CD	GLN	37	41.820	49.462	16.104	1.00	37.78	CPS3
ATOM	2150	OE1	GLN	37	42.601	48.806	16.803	1.00	38.25	CPS3
ATOM	2151	NE2	GLN	37	42.233	50.256	15.128	1.00	40.09	CPS3
ATOM	2152	C	GLN	37	37.729	46.838	14.954	1.00	28.42	CPS3
ATOM	2153	O	GLN	37	37.107	47.097	13.918	1.00	28.25	CPS3
ATOM	2154	N	TYR	38	38.040	45.602	15.322	1.00	25.92	CPS3
ATOM	2155	CA	TYR	38	37.676	44.445	14.526	1.00	27.76	CPS3
ATOM	2156	CB	TYR	38	38.124	43.179	15.268	1.00	26.65	CPS3
ATOM	2157	CG	TYR	38	37.674	41.867	14.666	1.00	28.74	CPS3
ATOM	2158	CD1	TYR	38	36.522	41.225	15.130	1.00	27.49	CPS3
ATOM	2159	CE1	TYR	38	36.105	40.013	14.583	1.00	29.24	CPS3
ATOM	2160	CD2	TYR	38	38.397	41.264	13.636	1.00	27.76	CPS3
ATOM	2161	CE2	TYR	38	37.986	40.046	13.081	1.00	29.24	CPS3
ATOM	2162	CZ	TYR	38	36.840	39.430	13.565	1.00	29.43	CPS3
ATOM	2163	OH	TYR	38	36.440	38.218	13.057	1.00	30.36	CPS3
ATOM	2164	C	TYR	38	36.177	44.398	14.219	1.00	28.73	CPS3
ATOM	2165	O	TYR	38	35.776	44.169	13.075	1.00	28.54	CPS3

FIG. 1A-38

ATOM	2166	N	TYR	39	35.349	44.637	15.228	1.00	29.50	CPS3
ATOM	2167	CA	TYR	39	33.910	44.575	15.018	1.00	31.58	CPS3
ATOM	2168	CB	TYR	39	33.195	44.515	16.367	1.00	31.24	CPS3
ATOM	2169	CG	TYR	39	33.219	43.106	16.896	1.00	31.89	CPS3
ATOM	2170	CD1	TYR	39	32.839	42.054	16.068	1.00	34.16	CPS3
ATOM	2171	CE1	TYR	39	32.897	40.744	16.491	1.00	34.63	CPS3
ATOM	2172	CD2	TYR	39	33.658	42.808	18.185	1.00	32.76	CPS3
ATOM	2173	CE2	TYR	39	33.722	41.472	18.627	1.00	32.49	CPS3
ATOM	2174	CZ	TYR	39	33.339	40.455	17.760	1.00	33.06	CPS3
ATOM	2175	OH	TYR	39	33.404	39.126	18.112	1.00	36.81	CPS3
ATOM	2176	C	TYR	39	33.277	45.627	14.110	1.00	33.88	CPS3
ATOM	2177	O	TYR	39	32.122	45.484	13.715	1.00	34.54	CPS3
ATOM	2178	N	GLU	40	34.026	46.666	13.766	1.00	35.41	CPS3
ATOM	2179	CA	GLU	40	33.509	47.709	12.882	1.00	37.60	CPS3
ATOM	2180	CB	GLU	40	34.045	49.077	13.302	1.00	39.04	CPS3
ATOM	2181	CG	GLU	40	33.553	49.545	14.656	1.00	41.70	CPS3
ATOM	2182	CD	GLU	40	32.040	49.515	14.755	1.00	44.23	CPS3
ATOM	2183	OE1	GLU	40	31.374	50.110	13.879	1.00	46.21	CPS3
ATOM	2184	OE2	GLU	40	31.515	48.895	15.706	1.00	44.59	CPS3
ATOM	2185	C	GLU	40	33.888	47.452	11.423	1.00	38.62	CPS3
ATOM	2186	O	GLU	40	33.491	48.200	10.530	1.00	39.31	CPS3
ATOM	2187	N	LEU	41	34.651	46.388	11.189	1.00	38.25	CPS3
ATOM	2188	CA	LEU	41	35.120	46.028	9.851	1.00	37.52	CPS3
ATOM	2189	CB	LEU	41	36.507	45.380	9.954	1.00	36.60	CPS3
ATOM	2190	CG	LEU	41	37.764	46.251	10.003	1.00	37.26	CPS3
ATOM	2191	CD1	LEU	41	37.520	47.514	10.794	1.00	38.83	CPS3
ATOM	2192	CD2	LEU	41	38.906	45.436	10.604	1.00	35.48	CPS3
ATOM	2193	C	LEU	41	34.206	45.080	9.079	1.00	37.57	CPS3
ATOM	2194	O	LEU	41	33.441	44.317	9.662	1.00	36.05	CPS3
ATOM	2195	N	SER	42	34.312	45.127	7.755	1.00	38.63	CPS3
ATOM	2196	CA	SER	42	33.537	44.251	6.890	1.00	38.96	CPS3
ATOM	2197	CB	SER	42	33.712	44.668	5.434	1.00	40.14	CPS3
ATOM	2198	OG	SER	42	35.078	44.585	5.055	1.00	42.27	CPS3
ATOM	2199	C	SER	42	34.102	42.849	7.077	1.00	39.70	CPS3
ATOM	2200	O	SER	42	35.183	42.685	7.641	1.00	39.21	CPS3
ATOM	2201	N	ALA	43	33.385	41.842	6.596	1.00	39.38	CPS3
ATOM	2202	CA	ALA	43	33.844	40.463	6.721	1.00	40.19	CPS3
ATOM	2203	CB	ALA	43	32.854	39.521	6.040	1.00	41.29	CPS3
ATOM	2204	C	ALA	43	35.247	40.268	6.128	1.00	40.48	CPS3
ATOM	2205	O	ALA	43	36.084	39.569	6.706	1.00	39.82	CPS3
ATOM	2206	N	LYS	44	35.495	40.884	4.974	1.00	40.37	CPS3
ATOM	2207	CA	LYS	44	36.786	40.767	4.305	1.00	40.57	CPS3
ATOM	2208	CB	LYS	44	36.722	41.379	2.904	1.00	42.89	CPS3
ATOM	2209	CG	LYS	44	38.039	41.314	2.139	1.00	45.09	CPS3
ATOM	2210	CD	LYS	44	37.958	42.106	0.840	1.00	47.76	CPS3
ATOM	2211	CE	LYS	44	39.309	42.177	0.145	1.00	49.05	CPS3
ATOM	2212	NZ	LYS	44	39.300	43.158	-0.980	1.00	50.90	CPS3
ATOM	2213	C	LYS	44	37.886	41.454	5.097	1.00	39.09	CPS3
ATOM	2214	O	LYS	44	38.955	40.881	5.308	1.00	39.00	CPS3
ATOM	2215	N	ARG	45	37.625	42.687	5.518	1.00	37.74	CPS3
ATOM	2216	CA	ARG	45	38.594	43.460	6.291	1.00	36.13	CPS3
ATOM	2217	CB	ARG	45	38.073	44.882	6.517	1.00	37.61	CPS3
ATOM	2218	CG	ARG	45	38.223	45.805	5.314	1.00	41.25	CPS3
ATOM	2219	CD	ARG	45	39.693	46.134	5.076	1.00	43.51	CPS3
ATOM	2220	NE	ARG	45	40.264	46.872	6.203	1.00	45.35	CPS3
ATOM	2221	CZ	ARG	45	41.392	46.536	6.826	1.00	46.41	CPS3
ATOM	2222	NH1	ARG	45	42.078	45.469	6.435	1.00	46.39	CPS3

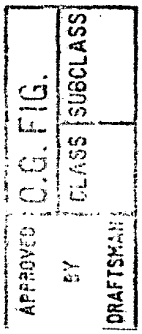
FIG. 1A-39

ATOM	2223	NH2	ARG	45	41.833	47.269	7.843	1.00	46.62	CPS3
ATOM	2224	C	ARG	45	38.909	42.799	7.634	1.00	34.32	CPS3
ATOM	2225	O	ARG	45	40.049	42.842	8.097	1.00	32.42	CPS3
ATOM	2226	N	LYS	46	37.899	42.188	8.251	1.00	32.83	CPS3
ATOM	2227	CA	LYS	46	38.075	41.509	9.532	1.00	31.12	CPS3
ATOM	2228	CB	LYS	46	36.775	40.842	9.987	1.00	31.02	CPS3
ATOM	2229	CG	LYS	46	35.746	41.775	10.599	1.00	30.98	CPS3
ATOM	2230	CD	LYS	46	34.553	40.977	11.100	1.00	32.86	CPS3
ATOM	2231	CE	LYS	46	33.524	41.861	11.785	1.00	34.98	CPS3
ATOM	2232	NZ	LYS	46	32.360	41.053	12.230	1.00	37.21	CPS3
ATOM	2233	C	LYS	46	39.148	40.438	9.434	1.00	30.57	CPS3
ATOM	2234	O	LYS	46	40.025	40.352	10.293	1.00	28.78	CPS3
ATOM	2235	N	ASN	47	39.061	39.612	8.392	1.00	29.54	CPS3
ATOM	2236	CA	ASN	47	40.020	38.533	8.186	1.00	29.84	CPS3
ATOM	2237	CB	ASN	47	39.589	37.671	6.989	1.00	31.31	CPS3
ATOM	2238	CG	ASN	47	40.603	36.588	6.635	1.00	33.49	CPS3
ATOM	2239	OD1	ASN	47	40.838	35.651	7.400	1.00	34.63	CPS3
ATOM	2240	ND2	ASN	47	41.201	36.713	5.461	1.00	34.30	CPS3
ATOM	2241	C	ASN	47	41.436	39.083	7.976	1.00	28.84	CPS3
ATOM	2242	O	ASN	47	42.401	38.521	8.501	1.00	27.85	CPS3
ATOM	2243	N	GLU	48	41.562	40.174	7.224	1.00	27.20	CPS3
ATOM	2244	CA	GLU	48	42.881	40.779	6.988	1.00	27.86	CPS3
ATOM	2245	CB	GLU	48	42.795	41.910	5.955	1.00	30.08	CPS3
ATOM	2246	CG	GLU	48	42.315	41.492	4.580	1.00	34.36	CPS3
ATOM	2247	CD	GLU	48	41.937	42.687	3.716	1.00	38.77	CPS3
ATOM	2248	OE1	GLU	48	41.356	42.477	2.627	1.00	40.99	CPS3
ATOM	2249	OE2	GLU	48	42.221	43.835	4.124	1.00	39.72	CPS3
ATOM	2250	C	GLU	48	43.451	41.363	8.285	1.00	25.90	CPS3
ATOM	2251	O	GLU	48	44.633	41.197	8.589	1.00	24.51	CPS3
ATOM	2252	N	PHE	49	42.601	42.065	9.030	1.00	24.05	CPS3
ATOM	2253	CA	PHE	49	42.995	42.688	10.293	1.00	24.45	CPS3
ATOM	2254	CB	PHE	49	41.809	43.473	10.866	1.00	25.52	CPS3
ATOM	2255	CG	PHE	49	42.073	44.119	12.203	1.00	26.02	CPS3
ATOM	2256	CD1	PHE	49	42.503	45.440	12.285	1.00	26.53	CPS3
ATOM	2257	CD2	PHE	49	41.842	43.419	13.385	1.00	26.09	CPS3
ATOM	2258	CE1	PHE	49	42.688	46.061	13.529	1.00	26.57	CPS3
ATOM	2259	CE2	PHE	49	42.028	44.027	14.630	1.00	25.34	CPS3
ATOM	2260	CZ	PHE	49	42.448	45.350	14.702	1.00	24.86	CPS3
ATOM	2261	C	PHE	49	43.431	41.603	11.278	1.00	24.05	CPS3
ATOM	2262	O	PHE	49	44.499	41.691	11.885	1.00	22.16	CPS3
ATOM	2263	N	LEU	50	42.597	40.577	11.429	1.00	23.09	CPS3
ATOM	2264	CA	LEU	50	42.894	39.478	12.342	1.00	23.23	CPS3
ATOM	2265	CB	LEU	50	41.727	38.488	12.348	1.00	24.42	CPS3
ATOM	2266	CG	LEU	50	41.788	37.294	13.297	1.00	26.20	CPS3
ATOM	2267	CD1	LEU	50	42.039	37.735	14.751	1.00	26.62	CPS3
ATOM	2268	CD2	LEU	50	40.468	36.551	13.182	1.00	27.72	CPS3
ATOM	2269	C	LEU	50	44.191	38.758	11.970	1.00	22.25	CPS3
ATOM	2270	O	LEU	50	45.033	38.483	12.835	1.00	21.88	CPS3
ATOM	2271	N	ALA	51	44.359	38.455	10.685	1.00	21.04	CPS3
ATOM	2272	CA	ALA	51	45.564	37.773	10.223	1.00	20.88	CPS3
ATOM	2273	CB	ALA	51	45.460	37.467	8.727	1.00	21.96	CPS3
ATOM	2274	C	ALA	51	46.815	38.615	10.497	1.00	21.09	CPS3
ATOM	2275	O	ALA	51	47.860	38.077	10.863	1.00	20.76	CPS3
ATOM	2276	N	GLY	52	46.698	39.929	10.321	1.00	21.47	CPS3
ATOM	2277	CA	GLY	52	47.830	40.814	10.559	1.00	20.85	CPS3
ATOM	2278	C	GLY	52	48.230	40.871	12.026	1.00	21.87	CPS3
ATOM	2279	O	GLY	52	49.420	40.891	12.355	1.00	20.94	CPS3

FIG. 1A-40

ATOM	2280	N	ARG	53	47.234	40.907	12.908	1.00	20.71	CPS3
ATOM	2281	CA	ARG	53	47.489	40.953	14.344	1.00	19.99	CPS3
ATOM	2282	CB	ARG	53	46.188	41.249	15.102	1.00	21.12	CPS3
ATOM	2283	CG	ARG	53	45.749	42.697	15.023	1.00	25.14	CPS3
ATOM	2284	CD	ARG	53	46.854	43.589	15.542	1.00	26.59	CPS3
ATOM	2285	NE	ARG	53	46.364	44.864	16.046	1.00	29.01	CPS3
ATOM	2286	CZ	ARG	53	46.020	45.905	15.293	1.00	29.46	CPS3
ATOM	2287	NH1	ARG	53	46.104	45.841	13.967	1.00	29.27	CPS3
ATOM	2288	NH2	ARG	53	45.615	47.028	15.882	1.00	26.91	CPS3
ATOM	2289	C	ARG	53	48.067	39.628	14.802	1.00	18.67	CPS3
ATOM	2290	O	ARG	53	48.983	39.585	15.623	1.00	19.03	CPS3
ATOM	2291	N	PHE	54	47.524	38.541	14.274	1.00	19.10	CPS3
ATOM	2292	CA	PHE	54	48.001	37.214	14.639	1.00	18.17	CPS3
ATOM	2293	CB	PHE	54	47.145	36.157	13.926	1.00	20.62	CPS3
ATOM	2294	CG	PHE	54	47.514	34.736	14.248	1.00	21.61	CPS3
ATOM	2295	CD1	PHE	54	48.429	34.050	13.462	1.00	22.92	CPS3
ATOM	2296	CD2	PHE	54	46.903	34.068	15.305	1.00	23.51	CPS3
ATOM	2297	CE1	PHE	54	48.731	32.726	13.713	1.00	24.49	CPS3
ATOM	2298	CE2	PHE	54	47.196	32.735	15.572	1.00	24.31	CPS3
ATOM	2299	CZ	PHE	54	48.113	32.061	14.773	1.00	26.02	CPS3
ATOM	2300	C	PHE	54	49.480	37.082	14.254	1.00	18.48	CPS3
ATOM	2301	O	PHE	54	50.296	36.615	15.049	1.00	16.83	CPS3
ATOM	2302	N	ALA	55	49.818	37.512	13.042	1.00	18.82	CPS3
ATOM	2303	CA	ALA	55	51.202	37.426	12.564	1.00	19.23	CPS3
ATOM	2304	CB	ALA	55	51.291	37.903	11.110	1.00	19.19	CPS3
ATOM	2305	C	ALA	55	52.121	38.271	13.439	1.00	17.75	CPS3
ATOM	2306	O	ALA	55	53.210	37.833	13.822	1.00	17.44	CPS3
ATOM	2307	N	ALA	56	51.678	39.481	13.755	1.00	17.64	CPS3
ATOM	2308	CA	ALA	56	52.490	40.382	14.572	1.00	17.27	CPS3
ATOM	2309	CB	ALA	56	51.828	41.769	14.651	1.00	17.54	CPS3
ATOM	2310	C	ALA	56	52.745	39.840	15.978	1.00	18.48	CPS3
ATOM	2311	O	ALA	56	53.869	39.927	16.492	1.00	16.93	CPS3
ATOM	2312	N	LYS	57	51.710	39.278	16.600	1.00	17.56	CPS3
ATOM	2313	CA	LYS	57	51.864	38.758	17.953	1.00	17.39	CPS3
ATOM	2314	CB	LYS	57	50.484	38.545	18.593	1.00	17.01	CPS3
ATOM	2315	CG	LYS	57	49.741	39.852	18.728	1.00	17.00	CPS3
ATOM	2316	CD	LYS	57	48.445	39.709	19.516	1.00	17.39	CPS3
ATOM	2317	CE	LYS	57	47.650	41.015	19.466	1.00	17.65	CPS3
ATOM	2318	NZ	LYS	57	46.589	41.049	20.526	1.00	18.42	CPS3
ATOM	2319	C	LYS	57	52.694	37.492	17.958	1.00	18.30	CPS3
ATOM	2320	O	LYS	57	53.456	37.248	18.895	1.00	17.97	CPS3
ATOM	2321	N	GLU	58	52.555	36.692	16.903	1.00	19.29	CPS3
ATOM	2322	CA	GLU	58	53.343	35.477	16.770	1.00	21.29	CPS3
ATOM	2323	CB	GLU	58	52.885	34.710	15.518	1.00	25.54	CPS3
ATOM	2324	CG	GLU	58	52.985	33.214	15.639	1.00	35.02	CPS3
ATOM	2325	CD	GLU	58	52.321	32.682	16.899	1.00	36.12	CPS3
ATOM	2326	OE1	GLU	58	51.079	32.744	17.033	1.00	40.18	CPS3
ATOM	2327	OE2	GLU	58	53.059	32.207	17.772	1.00	38.83	CPS3
ATOM	2328	C	GLU	58	54.818	35.900	16.644	1.00	20.21	CPS3
ATOM	2329	O	GLU	58	55.696	35.365	17.335	1.00	19.40	CPS3
ATOM	2330	N	ALA	59	55.089	36.867	15.768	1.00	16.40	CPS3
ATOM	2331	CA	ALA	59	56.458	37.353	15.580	1.00	17.36	CPS3
ATOM	2332	CB	ALA	59	56.491	38.461	14.521	1.00	17.44	CPS3
ATOM	2333	C	ALA	59	57.011	37.883	16.900	1.00	17.42	CPS3
ATOM	2334	O	ALA	59	58.160	37.595	17.271	1.00	17.74	CPS3
ATOM	2335	N	PHE	60	56.200	38.657	17.613	1.00	16.51	CPS3
ATOM	2336	CA	PHE	60	56.655	39.219	18.882	1.00	17.55	CPS3

FIG. 1A-41



ATOM	2337	CB	PHE	60	55.586	40.128	19.502	1.00	17.91	CPS3
ATOM	2338	CG	PHE	60	55.984	40.684	20.847	1.00	18.76	CPS3
ATOM	2339	CD1	PHE	60	56.755	41.838	20.933	1.00	18.58	CPS3
ATOM	2340	CD2	PHE	60	55.659	40.001	22.021	1.00	19.49	CPS3
ATOM	2341	CE1	PHE	60	57.212	42.309	22.172	1.00	20.20	CPS3
ATOM	2342	CE2	PHE	60	56.107	40.459	23.266	1.00	20.93	CPS3
ATOM	2343	CZ	PHE	60	56.886	41.612	23.341	1.00	20.99	CPS3
ATOM	2344	C	PHE	60	57.008	38.118	19.883	1.00	18.91	CPS3
ATOM	2345	O	PHE	60	58.053	38.173	20.543	1.00	18.95	CPS3
ATOM	2346	N	SER	61	56.137	37.123	20.001	1.00	18.23	CPS3
ATOM	2347	CA	SER	61	56.370	36.036	20.946	1.00	19.91	CPS3
ATOM	2348	CB	SER	61	55.167	35.081	20.978	1.00	20.94	CPS3
ATOM	2349	OG	SER	61	55.170	34.217	19.851	1.00	25.41	CPS3
ATOM	2350	C	SER	61	57.642	35.256	20.618	1.00	21.39	CPS3
ATOM	2351	O	SER	61	58.278	34.697	21.511	1.00	21.46	CPS3
ATOM	2352	N	LYS	62	58.011	35.206	19.345	1.00	20.86	CPS3
ATOM	2353	CA	LYS	62	59.227	34.500	18.958	1.00	23.14	CPS3
ATOM	2354	CB	LYS	62	59.239	34.237	17.455	1.00	24.31	CPS3
ATOM	2355	CG	LYS	62	58.295	33.143	17.003	1.00	28.06	CPS3
ATOM	2356	CD	LYS	62	58.340	33.057	15.490	1.00	32.02	CPS3
ATOM	2357	CE	LYS	62	58.060	31.655	14.987	1.00	34.92	CPS3
ATOM	2358	NZ	LYS	62	58.159	31.623	13.510	1.00	35.49	CPS3
ATOM	2359	C	LYS	62	60.444	35.343	19.340	1.00	22.30	CPS3
ATOM	2360	O	LYS	62	61.464	34.815	19.788	1.00	23.20	CPS3
ATOM	2361	N	ALA	63	60.337	36.654	19.156	1.00	19.62	CPS3
ATOM	2362	CA	ALA	63	61.437	37.547	19.512	1.00	20.06	CPS3
ATOM	2363	CB	ALA	63	61.145	38.960	19.019	1.00	20.10	CPS3
ATOM	2364	C	ALA	63	61.603	37.543	21.035	1.00	21.63	CPS3
ATOM	2365	O	ALA	63	62.724	37.529	21.550	1.00	23.66	CPS3
ATOM	2366	N	PHE	64	60.480	37.536	21.749	1.00	20.52	CPS3
ATOM	2367	CA	PHE	64	60.502	37.548	23.209	1.00	23.24	CPS3
ATOM	2368	CB	PHE	64	59.079	37.690	23.752	1.00	23.53	CPS3
ATOM	2369	CG	PHE	64	59.023	38.051	25.211	1.00	24.99	CPS3
ATOM	2370	CD1	PHE	64	59.492	39.283	25.653	1.00	26.02	CPS3
ATOM	2371	CD2	PHE	64	58.488	37.163	26.135	1.00	25.12	CPS3
ATOM	2372	CE1	PHE	64	59.423	39.632	27.008	1.00	28.33	CPS3
ATOM	2373	CE2	PHE	64	58.412	37.495	27.484	1.00	26.52	CPS3
ATOM	2374	CZ	PHE	64	58.877	38.729	27.924	1.00	27.24	CPS3
ATOM	2375	C	PHE	64	61.140	36.251	23.718	1.00	25.44	CPS3
ATOM	2376	O	PHE	64	61.688	36.204	24.826	1.00	24.64	CPS3
ATOM	2377	N	GLY	65	61.039	35.202	22.910	1.00	26.62	CPS3
ATOM	2378	CA	GLY	65	61.662	33.938	23.255	1.00	30.83	CPS3
ATOM	2379	C	GLY	65	60.802	32.879	23.912	1.00	32.24	CPS3
ATOM	2380	O	GLY	65	61.209	31.719	23.980	1.00	33.69	CPS3
ATOM	2381	N	THR	66	59.616	33.256	24.376	1.00	32.78	CPS3
ATOM	2382	CA	THR	66	58.733	32.302	25.043	1.00	34.27	CPS3
ATOM	2383	CB	THR	66	57.991	32.969	26.200	1.00	35.66	CPS3
ATOM	2384	OG1	THR	66	57.122	33.978	25.668	1.00	37.64	CPS3
ATOM	2385	CG2	THR	66	58.969	33.610	27.179	1.00	34.33	CPS3
ATOM	2386	C	THR	66	57.663	31.691	24.143	1.00	34.55	CPS3
ATOM	2387	O	THR	66	57.154	30.610	24.431	1.00	34.19	CPS3
ATOM	2388	N	GLY	67	57.320	32.376	23.054	1.00	34.33	CPS3
ATOM	2389	CA	GLY	67	56.256	31.877	22.198	1.00	34.53	CPS3
ATOM	2390	C	GLY	67	54.962	32.175	22.945	1.00	34.85	CPS3
ATOM	2391	O	GLY	67	55.012	32.656	24.080	1.00	34.24	CPS3
ATOM	2392	N	ILE	68	53.808	31.915	22.338	1.00	35.31	CPS3
ATOM	2393	CA	ILE	68	52.537	32.175	23.016	1.00	35.28	CPS3

FIG. 1A-42

ATOM	2394	CB	ILE	68	51.389	32.407	22.011	1.00 34.11	CPS3
ATOM	2395	CG2	ILE	68	50.052	32.474	22.755	1.00 32.62	CPS3
ATOM	2396	CG1	ILE	68	51.640	33.690	21.219	1.00 32.54	CPS3
ATOM	2397	CD1	ILE	68	51.647	34.958	22.063	1.00 32.72	CPS3
ATOM	2398	C	ILE	68	52.161	30.999	23.910	1.00 36.56	CPS3
ATOM	2399	O	ILE	68	52.085	29.862	23.447	1.00 36.53	CPS3
ATOM	2400	N	GLY	69	51.922	31.279	25.187	1.00 36.84	CPS3
ATOM	2401	CA	GLY	69	51.565	30.221	26.115	1.00 38.40	CPS3
ATOM	2402	C	GLY	69	51.481	30.700	27.550	1.00 38.69	CPS3
ATOM	2403	O	GLY	69	50.987	31.797	27.820	1.00 38.83	CPS3
ATOM	2404	N	ALA	70	51.978	29.882	28.474	1.00 38.37	CPS3
ATOM	2405	CA	ALA	70	51.949	30.215	29.895	1.00 37.89	CPS3
ATOM	2406	CB	ALA	70	52.510	29.043	30.710	1.00 38.76	CPS3
ATOM	2407	C	ALA	70	52.684	31.506	30.270	1.00 37.56	CPS3
ATOM	2408	O	ALA	70	52.225	32.262	31.122	1.00 37.72	CPS3
ATOM	2409	N	GLN	71	53.817	31.769	29.634	1.00 36.91	CPS3
ATOM	2410	CA	GLN	71	54.590	32.965	29.954	1.00 36.41	CPS3
ATOM	2411	CB	GLN	71	56.072	32.693	29.697	1.00 38.98	CPS3
ATOM	2412	CG	GLN	71	56.540	31.358	30.251	1.00 42.83	CPS3
ATOM	2413	CD	GLN	71	58.024	31.132	30.053	1.00 45.56	CPS3
ATOM	2414	OE1	GLN	71	58.854	31.783	30.695	1.00 47.59	CPS3
ATOM	2415	NE2	GLN	71	58.369	30.211	29.156	1.00 47.26	CPS3
ATOM	2416	C	GLN	71	54.167	34.225	29.192	1.00 33.99	CPS3
ATOM	2417	O	GLN	71	54.514	35.332	29.585	1.00 34.52	CPS3
ATOM	2418	N	LEU	72	53.422	34.056	28.107	1.00 30.98	CPS3
ATOM	2419	CA	LEU	72	52.993	35.195	27.304	1.00 27.97	CPS3
ATOM	2420	CB	LEU	72	54.108	35.592	26.333	1.00 26.71	CPS3
ATOM	2421	CG	LEU	72	53.888	36.797	25.415	1.00 25.21	CPS3
ATOM	2422	CD1	LEU	72	54.008	38.103	26.212	1.00 25.07	CPS3
ATOM	2423	CD2	LEU	72	54.930	36.760	24.299	1.00 26.26	CPS3
ATOM	2424	C	LEU	72	51.727	34.852	26.532	1.00 26.94	CPS3
ATOM	2425	O	LEU	72	51.679	33.877	25.779	1.00 27.79	CPS3
ATOM	2426	N	SER	73	50.706	35.673	26.723	1.00 24.63	CPS3
ATOM	2427	CA	SER	73	49.416	35.486	26.081	1.00 24.89	CPS3
ATOM	2428	CB	SER	73	48.318	35.677	27.135	1.00 26.50	CPS3
ATOM	2429	OG	SER	73	47.068	35.913	26.531	1.00 28.99	CPS3
ATOM	2430	C	SER	73	49.228	36.504	24.957	1.00 23.56	CPS3
ATOM	2431	O	SER	73	49.903	37.537	24.942	1.00 22.03	CPS3
ATOM	2432	N	PHE	74	48.324	36.211	24.017	1.00 22.96	CPS3
ATOM	2433	CA	PHE	74	48.016	37.150	22.933	1.00 21.51	CPS3
ATOM	2434	CB	PHE	74	46.922	36.599	22.010	1.00 23.03	CPS3
ATOM	2435	CG	PHE	74	47.386	35.535	21.060	1.00 24.56	CPS3
ATOM	2436	CD1	PHE	74	48.330	35.820	20.079	1.00 25.15	CPS3
ATOM	2437	CD2	PHE	74	46.854	34.246	21.127	1.00 26.66	CPS3
ATOM	2438	CE1	PHE	74	48.740	34.837	19.175	1.00 25.67	CPS3
ATOM	2439	CE2	PHE	74	47.257	33.251	20.226	1.00 27.19	CPS3
ATOM	2440	CZ	PHE	74	48.200	33.547	19.251	1.00 26.99	CPS3
ATOM	2441	C	PHE	74	47.476	38.424	23.573	1.00 22.00	CPS3
ATOM	2442	O	PHE	74	47.624	39.519	23.038	1.00 20.92	CPS3
ATOM	2443	N	GLN	75	46.830	38.270	24.726	1.00 22.26	CPS3
ATOM	2444	CA	GLN	75	46.246	39.402	25.431	1.00 22.41	CPS3
ATOM	2445	CB	GLN	75	45.313	38.895	26.543	1.00 23.41	CPS3
ATOM	2446	CG	GLN	75	44.119	38.109	26.025	1.00 25.20	CPS3
ATOM	2447	CD	GLN	75	43.257	38.954	25.118	1.00 26.61	CPS3
ATOM	2448	OE1	GLN	75	42.891	40.080	25.476	1.00 27.48	CPS3
ATOM	2449	NE2	GLN	75	42.928	38.429	23.938	1.00 25.82	CPS3
ATOM	2450	C	GLN	75	47.287	40.350	26.028	1.00 22.75	CPS3

FIG. 1A-43

ATOM	2451	O	GLN	75	46.962	41.486	26.389	1.00	21.60	CPS3
ATOM	2452	N	ASP	76	48.532	39.890	26.146	1.00	21.97	CPS3
ATOM	2453	CA	ASP	76	49.595	40.730	26.710	1.00	22.16	CPS3
ATOM	2454	CB	ASP	76	50.738	39.876	27.279	1.00	22.82	CPS3
ATOM	2455	CG	ASP	76	50.332	39.058	28.494	1.00	25.52	CPS3
ATOM	2456	OD1	ASP	76	49.557	39.565	29.332	1.00	25.20	CPS3
ATOM	2457	OD2	ASP	76	50.823	37.915	28.614	1.00	24.81	CPS3
ATOM	2458	C	ASP	76	50.223	41.635	25.661	1.00	21.66	CPS3
ATOM	2459	O	ASP	76	51.059	42.481	25.982	1.00	19.63	CPS3
ATOM	2460	N	ILE	77	49.826	41.450	24.405	1.00	21.29	CPS3
ATOM	2461	CA	ILE	77	50.416	42.202	23.301	1.00	19.67	CPS3
ATOM	2462	CB	ILE	77	51.088	41.225	22.318	1.00	19.23	CPS3
ATOM	2463	CG2	ILE	77	51.893	41.995	21.253	1.00	18.53	CPS3
ATOM	2464	CG1	ILE	77	51.987	40.247	23.084	1.00	17.28	CPS3
ATOM	2465	CD1	ILE	77	52.313	38.989	22.257	1.00	19.10	CPS3
ATOM	2466	C	ILE	77	49.379	42.988	22.520	1.00	20.27	CPS3
ATOM	2467	O	ILE	77	48.401	42.416	22.062	1.00	20.00	CPS3
ATOM	2468	N	GLU	78	49.603	44.288	22.354	1.00	21.09	CPS3
ATOM	2469	CA	GLU	78	48.670	45.106	21.591	1.00	20.73	CPS3
ATOM	2470	CB	GLU	78	47.909	46.082	22.496	1.00	22.17	CPS3
ATOM	2471	CG	GLU	78	46.819	46.843	21.737	1.00	24.01	CPS3
ATOM	2472	CD	GLU	78	45.862	47.584	22.651	1.00	27.03	CPS3
ATOM	2473	OE1	GLU	78	46.036	48.806	22.844	1.00	28.55	CPS3
ATOM	2474	OE2	GLU	78	44.937	46.934	23.181	1.00	28.54	CPS3
ATOM	2475	C	GLU	78	49.384	45.892	20.508	1.00	20.37	CPS3
ATOM	2476	O	GLU	78	50.431	46.485	20.749	1.00	20.67	CPS3
ATOM	2477	N	ILE	79	48.826	45.877	19.303	1.00	19.96	CPS3
ATOM	2478	CA	ILE	79	49.420	46.642	18.212	1.00	19.14	CPS3
ATOM	2479	CB	ILE	79	49.368	45.860	16.850	1.00	19.23	CPS3
ATOM	2480	CG2	ILE	79	49.577	46.830	15.678	1.00	19.82	CPS3
ATOM	2481	CG1	ILE	79	50.477	44.798	16.795	1.00	21.31	CPS3
ATOM	2482	CD1	ILE	79	50.318	43.645	17.758	1.00	22.36	CPS3
ATOM	2483	C	ILE	79	48.629	47.942	18.090	1.00	20.00	CPS3
ATOM	2484	O	ILE	79	47.389	47.928	18.088	1.00	20.09	CPS3
ATOM	2485	N	ARG	80	49.340	49.068	18.028	1.00	19.20	CPS3
ATOM	2486	CA	ARG	80	48.703	50.380	17.861	1.00	20.32	CPS3
ATOM	2487	CB	ARG	80	48.924	51.258	19.107	1.00	20.53	CPS3
ATOM	2488	CG	ARG	80	48.340	50.644	20.380	1.00	21.77	CPS3
ATOM	2489	CD	ARG	80	48.505	51.527	21.617	1.00	23.01	CPS3
ATOM	2490	NE	ARG	80	47.957	50.833	22.780	1.00	23.15	CPS3
ATOM	2491	CZ	ARG	80	48.032	51.267	24.038	1.00	25.30	CPS3
ATOM	2492	NH1	ARG	80	48.634	52.412	24.321	1.00	20.84	CPS3
ATOM	2493	NH2	ARG	80	47.511	50.536	25.014	1.00	26.37	CPS3
ATOM	2494	C	ARG	80	49.349	51.037	16.640	1.00	20.88	CPS3
ATOM	2495	O	ARG	80	50.362	50.550	16.138	1.00	20.01	CPS3
ATOM	2496	N	LYS	81	48.755	52.123	16.148	1.00	21.43	CPS3
ATOM	2497	CA	LYS	81	49.316	52.839	14.998	1.00	22.45	CPS3
ATOM	2498	CB	LYS	81	48.327	52.868	13.829	1.00	25.71	CPS3
ATOM	2499	CG	LYS	81	47.907	51.512	13.309	1.00	31.70	CPS3
ATOM	2500	CD	LYS	81	49.057	50.788	12.665	1.00	34.29	CPS3
ATOM	2501	CE	LYS	81	48.582	49.508	11.996	1.00	36.91	CPS3
ATOM	2502	NZ	LYS	81	47.631	49.799	10.888	1.00	38.59	CPS3
ATOM	2503	C	LYS	81	49.591	54.269	15.423	1.00	22.25	CPS3
ATOM	2504	O	LYS	81	48.757	54.882	16.095	1.00	21.74	CPS3
ATOM	2505	N	ASP	82	50.750	54.801	15.048	1.00	21.32	CPS3
ATOM	2506	CA	ASP	82	51.055	56.169	15.411	1.00	24.29	CPS3
ATOM	2507	CB	ASP	82	52.568	56.396	15.564	1.00	23.73	CPS3

FIG. 1A-44

ATOM	2508	CG	ASP	82	53.340	56.303	14.253	1.00	25.37	CPS3
ATOM	2509	OD1	ASP	82	52.736	56.371	13.161	1.00	25.70	CPS3
ATOM	2510	OD2	ASP	82	54.585	56.182	14.331	1.00	27.40	CPS3
ATOM	2511	C	ASP	82	50.446	57.129	14.394	1.00	26.03	CPS3
ATOM	2512	O	ASP	82	49.682	56.711	13.518	1.00	25.08	CPS3
ATOM	2513	N	GLN	83	50.783	58.406	14.521	1.00	27.30	CPS3
ATOM	2514	CA	GLN	83	50.243	59.439	13.648	1.00	30.37	CPS3
ATOM	2515	CB	GLN	83	50.694	60.810	14.158	1.00	32.92	CPS3
ATOM	2516	CG	GLN	83	50.035	61.193	15.481	1.00	36.66	CPS3
ATOM	2517	CD	GLN	83	48.633	61.738	15.292	1.00	40.09	CPS3
ATOM	2518	OE1	GLN	83	48.448	62.940	15.079	1.00	42.06	CPS3
ATOM	2519	NE2	GLN	83	47.637	60.859	15.354	1.00	40.07	CPS3
ATOM	2520	C	GLN	83	50.587	59.276	12.167	1.00	30.09	CPS3
ATOM	2521	O	GLN	83	49.900	59.834	11.308	1.00	30.34	CPS3
ATOM	2522	N	ASN	84	51.647	58.532	11.865	1.00	29.03	CPS3
ATOM	2523	CA	ASN	84	52.024	58.296	10.471	1.00	29.59	CPS3
ATOM	2524	CB	ASN	84	53.544	58.202	10.303	1.00	31.65	CPS3
ATOM	2525	CG	ASN	84	54.239	59.536	10.457	1.00	34.87	CPS3
ATOM	2526	OD1	ASN	84	53.732	60.566	10.022	1.00	36.47	CPS3
ATOM	2527	ND2	ASN	84	55.425	59.520	11.060	1.00	36.00	CPS3
ATOM	2528	C	ASN	84	51.419	56.990	9.974	1.00	28.93	CPS3
ATOM	2529	O	ASN	84	51.609	56.613	8.815	1.00	30.32	CPS3
ATOM	2530	N	GLY	85	50.712	56.286	10.852	1.00	26.33	CPS3
ATOM	2531	CA	GLY	85	50.116	55.019	10.464	1.00	24.71	CPS3
ATOM	2532	C	GLY	85	51.063	53.851	10.697	1.00	23.82	CPS3
ATOM	2533	O	GLY	85	50.759	52.713	10.341	1.00	24.11	CPS3
ATOM	2534	N	LYS	86	52.214	54.131	11.302	1.00	21.10	CPS3
ATOM	2535	CA	LYS	86	53.204	53.096	11.582	1.00	21.62	CPS3
ATOM	2536	CB	LYS	86	54.561	53.738	11.883	1.00	21.42	CPS3
ATOM	2537	CG	LYS	86	55.625	52.760	12.401	1.00	23.00	CPS3
ATOM	2538	CD	LYS	86	56.097	51.789	11.325	1.00	22.60	CPS3
ATOM	2539	CE	LYS	86	57.073	50.766	11.921	1.00	21.76	CPS3
ATOM	2540	NZ	LYS	86	57.761	49.970	10.852	1.00	21.43	CPS3
ATOM	2541	C	LYS	86	52.782	52.244	12.783	1.00	20.36	CPS3
ATOM	2542	O	LYS	86	52.468	52.776	13.843	1.00	20.19	CPS3
ATOM	2543	N	PRO	87	52.770	50.912	12.632	1.00	20.59	CPS3
ATOM	2544	CD	PRO	87	52.925	50.084	11.423	1.00	21.13	CPS3
ATOM	2545	CA	PRO	87	52.375	50.091	13.781	1.00	20.38	CPS3
ATOM	2546	CB	PRO	87	52.082	48.729	13.160	1.00	22.01	CPS3
ATOM	2547	CG	PRO	87	53.044	48.675	12.009	1.00	23.44	CPS3
ATOM	2548	C	PRO	87	53.481	49.991	14.812	1.00	18.94	CPS3
ATOM	2549	O	PRO	87	54.662	49.996	14.468	1.00	18.59	CPS3
ATOM	2550	N	TYR	88	53.092	49.938	16.082	1.00	18.68	CPS3
ATOM	2551	CA	TYR	88	54.064	49.757	17.155	1.00	18.87	CPS3
ATOM	2552	CB	TYR	88	54.566	51.093	17.734	1.00	19.03	CPS3
ATOM	2553	CG	TYR	88	53.531	51.940	18.426	1.00	19.37	CPS3
ATOM	2554	CD1	TYR	88	53.395	51.915	19.804	1.00	19.95	CPS3
ATOM	2555	CE1	TYR	88	52.413	52.683	20.449	1.00	20.13	CPS3
ATOM	2556	CD2	TYR	88	52.665	52.756	17.693	1.00	19.40	CPS3
ATOM	2557	CE2	TYR	88	51.690	53.519	18.315	1.00	19.13	CPS3
ATOM	2558	CZ	TYR	88	51.562	53.479	19.691	1.00	18.55	CPS3
ATOM	2559	OH	TYR	88	50.568	54.204	20.299	1.00	19.71	CPS3
ATOM	2560	C	TYR	88	53.385	48.899	18.211	1.00	18.42	CPS3
ATOM	2561	O	TYR	88	52.159	48.825	18.277	1.00	18.60	CPS3
ATOM	2562	N	ILE	89	54.196	48.233	19.020	1.00	17.79	CPS3
ATOM	2563	CA	ILE	89	53.675	47.331	20.022	1.00	18.21	CPS3
ATOM	2564	CB	ILE	89	54.406	45.966	19.939	1.00	17.33	CPS3

FIG. 1A-45

ATOM	2565	CG2	ILE	89	54.146	45.145	21.217	1.00	18.20	CPS3
ATOM	2566	CG1	ILE	89	53.938	45.192	18.696	1.00	18.54	CPS3
ATOM	2567	CD1	ILE	89	54.805	43.948	18.365	1.00	18.01	CPS3
ATOM	2568	C	ILE	89	53.775	47.829	21.450	1.00	18.41	CPS3
ATOM	2569	O	ILE	89	54.749	48.465	21.832	1.00	18.45	CPS3
ATOM	2570	N	ILE	90	52.737	47.539	22.221	1.00	19.17	CPS3
ATOM	2571	CA	ILE	90	52.722	47.852	23.645	1.00	20.34	CPS3
ATOM	2572	CB	ILE	90	51.485	48.700	24.062	1.00	21.03	CPS3
ATOM	2573	CG2	ILE	90	51.364	48.738	25.608	1.00	21.79	CPS3
ATOM	2574	CG1	ILE	90	51.605	50.128	23.516	1.00	21.44	CPS3
ATOM	2575	CD1	ILE	90	52.787	50.918	24.079	1.00	22.03	CPS3
ATOM	2576	C	ILE	90	52.618	46.483	24.314	1.00	20.90	CPS3
ATOM	2577	O	ILE	90	51.722	45.704	23.994	1.00	22.15	CPS3
ATOM	2578	N	CYS	91	53.557	46.177	25.208	1.00	21.50	CPS3
ATOM	2579	CA	CYS	91	53.565	44.918	25.968	1.00	22.56	CPS3
ATOM	2580	CB	CYS	91	54.379	43.834	25.252	1.00	22.42	CPS3
ATOM	2581	SG	CYS	91	54.522	42.300	26.235	1.00	25.18	CPS3
ATOM	2582	C	CYS	91	54.251	45.307	27.279	1.00	23.27	CPS3
ATOM	2583	O	CYS	91	55.450	45.584	27.292	1.00	23.16	CPS3
ATOM	2584	N	THR	92	53.500	45.337	28.372	1.00	26.40	CPS3
ATOM	2585	CA	THR	92	54.076	45.784	29.638	1.00	28.79	CPS3
ATOM	2586	CB	THR	92	52.983	46.002	30.713	1.00	29.85	CPS3
ATOM	2587	OG1	THR	92	52.347	44.760	31.033	1.00	31.45	CPS3
ATOM	2588	CG2	THR	92	51.934	46.993	30.195	1.00	30.30	CPS3
ATOM	2589	C	THR	92	55.203	44.945	30.217	1.00	30.27	CPS3
ATOM	2590	O	THR	92	55.787	45.313	31.237	1.00	29.37	CPS3
ATOM	2591	N	LYS	93	55.520	43.828	29.571	1.00	30.96	CPS3
ATOM	2592	CA	LYS	93	56.618	42.991	30.031	1.00	32.02	CPS3
ATOM	2593	CB	LYS	93	56.521	41.608	29.397	1.00	33.43	CPS3
ATOM	2594	CG	LYS	93	55.509	40.711	30.098	1.00	36.42	CPS3
ATOM	2595	CD	LYS	93	55.253	39.426	29.337	1.00	38.18	CPS3
ATOM	2596	CE	LYS	93	54.583	38.385	30.227	1.00	40.38	CPS3
ATOM	2597	NZ	LYS	93	53.482	38.941	31.059	1.00	41.16	CPS3
ATOM	2598	C	LYS	93	57.956	43.657	29.701	1.00	31.94	CPS3
ATOM	2599	O	LYS	93	58.998	43.287	30.233	1.00	32.81	CPS3
ATOM	2600	N	LEU	94	57.924	44.655	28.824	1.00	31.18	CPS3
ATOM	2601	CA	LEU	94	59.139	45.378	28.473	1.00	30.06	CPS3
ATOM	2602	CB	LEU	94	59.903	44.637	27.376	1.00	31.03	CPS3
ATOM	2603	CG	LEU	94	59.121	43.973	26.240	1.00	31.49	CPS3
ATOM	2604	CD1	LEU	94	58.228	44.977	25.551	1.00	33.11	CPS3
ATOM	2605	CD2	LEU	94	60.109	43.366	25.258	1.00	31.24	CPS3
ATOM	2606	C	LEU	94	58.822	46.801	28.042	1.00	29.42	CPS3
ATOM	2607	O	LEU	94	57.657	47.165	27.909	1.00	28.23	CPS3
ATOM	2608	N	SER	95	59.852	47.618	27.841	1.00	28.87	CPS3
ATOM	2609	CA	SER	95	59.616	48.993	27.423	1.00	29.31	CPS3
ATOM	2610	CB	SER	95	60.853	49.867	27.631	1.00	30.92	CPS3
ATOM	2611	OG	SER	95	60.671	51.106	26.950	1.00	31.74	CPS3
ATOM	2612	C	SER	95	59.244	49.062	25.953	1.00	28.31	CPS3
ATOM	2613	O	SER	95	59.835	48.376	25.127	1.00	27.86	CPS3
ATOM	2614	N	PRO	96	58.269	49.914	25.611	1.00	28.41	CPS3
ATOM	2615	CD	PRO	96	57.504	50.793	26.516	1.00	29.30	CPS3
ATOM	2616	CA	PRO	96	57.829	50.074	24.221	1.00	27.35	CPS3
ATOM	2617	CB	PRO	96	56.749	51.155	24.312	1.00	28.52	CPS3
ATOM	2618	CG	PRO	96	56.259	51.056	25.722	1.00	29.70	CPS3
ATOM	2619	C	PRO	96	58.997	50.532	23.344	1.00	26.87	CPS3
ATOM	2620	O	PRO	96	59.060	50.209	22.156	1.00	25.42	CPS3
ATOM	2621	N	ALA	97	59.922	51.283	23.940	1.00	26.21	CPS3

FIG. 1A-46

ATOM	2622	CA	ALA	97	61.073	51.804	23.203	1.00 26.00	CPS3
ATOM	2623	CB	ALA	97	61.821	52.824	24.060	1.00 28.49	CPS3
ATOM	2624	C	ALA	97	62.031	50.709	22.744	1.00 25.63	CPS3
ATOM	2625	O	ALA	97	62.858	50.921	21.858	1.00 24.95	CPS3
ATOM	2626	N	ALA	98	61.916	49.532	23.342	1.00 24.02	CPS3
ATOM	2627	CA	ALA	98	62.793	48.426	22.986	1.00 23.40	CPS3
ATOM	2628	CB	ALA	98	63.054	47.574	24.215	1.00 25.00	CPS3
ATOM	2629	C	ALA	98	62.208	47.553	21.880	1.00 22.32	CPS3
ATOM	2630	O	ALA	98	62.868	46.645	21.401	1.00 22.68	CPS3
ATOM	2631	N	VAL	99	60.979	47.842	21.460	1.00 21.24	CPS3
ATOM	2632	CA	VAL	99	60.330	47.004	20.457	1.00 19.35	CPS3
ATOM	2633	CB	VAL	99	58.965	46.511	20.982	1.00 19.94	CPS3
ATOM	2634	CG1	VAL	99	58.383	45.474	20.027	1.00 21.36	CPS3
ATOM	2635	CG2	VAL	99	59.125	45.930	22.376	1.00 23.27	CPS3
ATOM	2636	C	VAL	99	60.100	47.691	19.121	1.00 19.01	CPS3
ATOM	2637	O	VAL	99	59.758	48.865	19.083	1.00 19.19	CPS3
ATOM	2638	N	HIS	100	60.295	46.941	18.037	1.00 18.11	CPS3
ATOM	2639	CA	HIS	100	60.080	47.439	16.685	1.00 19.23	CPS3
ATOM	2640	CB	HIS	100	61.426	47.732	16.029	1.00 21.42	CPS3
ATOM	2641	CG	HIS	100	62.233	48.753	16.772	1.00 24.13	CPS3
ATOM	2642	CD2	HIS	100	63.223	48.613	17.686	1.00 25.59	CPS3
ATOM	2643	ND1	HIS	100	62.007	50.105	16.654	1.00 25.95	CPS3
ATOM	2644	CE1	HIS	100	62.825	50.758	17.463	1.00 26.97	CPS3
ATOM	2645	NE2	HIS	100	63.572	49.874	18.100	1.00 26.97	CPS3
ATOM	2646	C	HIS	100	59.343	46.348	15.919	1.00 18.08	CPS3
ATOM	2647	O	HIS	100	59.707	45.178	16.027	1.00 17.62	CPS3
ATOM	2648	N	VAL	101	58.313	46.731	15.161	1.00 17.20	CPS3
ATOM	2649	CA	VAL	101	57.525	45.765	14.382	1.00 16.42	CPS3
ATOM	2650	CB	VAL	101	56.149	45.472	15.080	1.00 16.35	CPS3
ATOM	2651	CG1	VAL	101	55.316	46.753	15.156	1.00 15.91	CPS3
ATOM	2652	CG2	VAL	101	55.364	44.375	14.330	1.00 17.27	CPS3
ATOM	2653	C	VAL	101	57.244	46.312	12.982	1.00 16.80	CPS3
ATOM	2654	O	VAL	101	57.325	47.515	12.754	1.00 15.86	CPS3
ATOM	2655	N	SER	102	56.948	45.414	12.046	1.00 16.94	CPS3
ATOM	2656	CA	SER	102	56.554	45.816	10.694	1.00 17.40	CPS3
ATOM	2657	CB	SER	102	57.733	45.889	9.723	1.00 18.13	CPS3
ATOM	2658	OG	SER	102	57.255	46.343	8.454	1.00 19.88	CPS3
ATOM	2659	C	SER	102	55.566	44.752	10.240	1.00 17.06	CPS3
ATOM	2660	O	SER	102	55.738	43.569	10.531	1.00 16.38	CPS3
ATOM	2661	N	ILE	103	54.508	45.180	9.562	1.00 16.71	CPS3
ATOM	2662	CA	ILE	103	53.476	44.259	9.109	1.00 16.77	CPS3
ATOM	2663	CB	ILE	103	52.138	44.533	9.851	1.00 19.32	CPS3
ATOM	2664	CG2	ILE	103	51.062	43.538	9.386	1.00 20.27	CPS3
ATOM	2665	CG1	ILE	103	52.340	44.398	11.366	1.00 18.63	CPS3
ATOM	2666	CD1	ILE	103	51.099	44.754	12.195	1.00 17.98	CPS3
ATOM	2667	C	ILE	103	53.261	44.475	7.615	1.00 17.09	CPS3
ATOM	2668	O	ILE	103	53.304	45.608	7.140	1.00 18.12	CPS3
ATOM	2669	N	THR	104	53.038	43.390	6.880	1.00 18.52	CPS3
ATOM	2670	CA	THR	104	52.802	43.475	5.438	1.00 19.66	CPS3
ATOM	2671	CB	THR	104	54.116	43.197	4.636	1.00 20.60	CPS3
ATOM	2672	OG1	THR	104	53.888	43.430	3.246	1.00 21.77	CPS3
ATOM	2673	CG2	THR	104	54.583	41.763	4.822	1.00 20.35	CPS3
ATOM	2674	C	THR	104	51.694	42.494	5.020	1.00 20.81	CPS3
ATOM	2675	O	THR	104	51.347	41.586	5.770	1.00 19.47	CPS3
ATOM	2676	N	HIS	105	51.142	42.688	3.825	1.00 21.19	CPS3
ATOM	2677	CA	HIS	105	50.066	41.838	3.320	1.00 23.77	CPS3
ATOM	2678	CB	HIS	105	48.701	42.514	3.515	1.00 25.55	CPS3

FIG. 1A-47

ATOM	2679	CG	HIS	105	48.344	42.814	4.937	1.00	30.17	CPS3
ATOM	2680	CD2	HIS	105	48.668	43.859	5.737	1.00	31.35	CPS3
ATOM	2681	ND1	HIS	105	47.507	42.008	5.676	1.00	31.23	CPS3
ATOM	2682	CE1	HIS	105	47.327	42.544	6.872	1.00	33.22	CPS3
ATOM	2683	NE2	HIS	105	48.020	43.668	6.935	1.00	32.63	CPS3
ATOM	2684	C	HIS	105	50.178	41.619	1.817	1.00	22.69	CPS3
ATOM	2685	O	HIS	105	50.784	42.413	1.105	1.00	22.84	CPS3
ATOM	2686	N	THR	106	49.565	40.536	1.359	1.00	24.26	CPS3
ATOM	2687	CA	THR	106	49.426	40.244	-0.066	1.00	25.12	CPS3
ATOM	2688	CB	THR	106	50.338	39.107	-0.598	1.00	25.65	CPS3
ATOM	2689	OG1	THR	106	49.928	37.848	-0.047	1.00	25.72	CPS3
ATOM	2690	CG2	THR	106	51.805	39.395	-0.275	1.00	24.63	CPS3
ATOM	2691	C	THR	106	47.970	39.769	-0.097	1.00	25.84	CPS3
ATOM	2692	O	THR	106	47.290	39.753	0.934	1.00	24.47	CPS3
ATOM	2693	N	ALA	107	47.484	39.388	-1.265	1.00	25.43	CPS3
ATOM	2694	CA	ALA	107	46.108	38.937	-1.362	1.00	26.46	CPS3
ATOM	2695	CB	ALA	107	45.790	38.570	-2.820	1.00	27.17	CPS3
ATOM	2696	C	ALA	107	45.812	37.750	-0.444	1.00	26.57	CPS3
ATOM	2697	O	ALA	107	44.769	37.707	0.213	1.00	27.71	CPS3
ATOM	2698	N	GLU	108	46.738	36.799	-0.384	1.00	26.04	CPS3
ATOM	2699	CA	GLU	108	46.542	35.594	0.404	1.00	25.62	CPS3
ATOM	2700	CB	GLU	108	46.833	34.374	-0.475	1.00	29.10	CPS3
ATOM	2701	CG	GLU	108	46.172	34.475	-1.846	1.00	35.56	CPS3
ATOM	2702	CD	GLU	108	46.174	33.171	-2.616	1.00	40.28	CPS3
ATOM	2703	OE1	GLU	108	47.145	32.395	-2.485	1.00	42.87	CPS3
ATOM	2704	OE2	GLU	108	45.201	32.932	-3.369	1.00	44.28	CPS3
ATOM	2705	C	GLU	108	47.325	35.460	1.706	1.00	25.50	CPS3
ATOM	2706	O	GLU	108	47.087	34.520	2.463	1.00	23.92	CPS3
ATOM	2707	N	TYR	109	48.239	36.389	1.978	1.00	23.47	CPS3
ATOM	2708	CA	TYR	109	49.048	36.281	3.189	1.00	22.84	CPS3
ATOM	2709	CB	TYR	109	50.471	35.833	2.822	1.00	23.00	CPS3
ATOM	2710	CG	TYR	109	50.552	34.480	2.176	1.00	23.82	CPS3
ATOM	2711	CD1	TYR	109	50.485	33.317	2.936	1.00	23.06	CPS3
ATOM	2712	CE1	TYR	109	50.532	32.063	2.334	1.00	24.49	CPS3
ATOM	2713	CD2	TYR	109	50.668	34.361	0.793	1.00	23.15	CPS3
ATOM	2714	CE2	TYR	109	50.710	33.122	0.184	1.00	24.59	CPS3
ATOM	2715	CZ	TYR	109	50.641	31.980	0.956	1.00	24.33	CPS3
ATOM	2716	OH	TYR	109	50.655	30.756	0.341	1.00	26.41	CPS3
ATOM	2717	C	TYR	109	49.187	37.551	4.000	1.00	21.41	CPS3
ATOM	2718	O	TYR	109	49.021	38.659	3.477	1.00	21.21	CPS3
ATOM	2719	N	ALA	110	49.478	37.366	5.293	1.00	19.67	CPS3
ATOM	2720	CA	ALA	110	49.781	38.470	6.204	1.00	19.04	CPS3
ATOM	2721	CB	ALA	110	48.753	38.588	7.334	1.00	18.93	CPS3
ATOM	2722	C	ALA	110	51.137	38.048	6.776	1.00	19.30	CPS3
ATOM	2723	O	ALA	110	51.375	36.861	6.985	1.00	20.91	CPS3
ATOM	2724	N	ALA	111	52.038	38.997	7.014	1.00	18.04	CPS3
ATOM	2725	CA	ALA	111	53.337	38.631	7.565	1.00	17.63	CPS3
ATOM	2726	CB	ALA	111	54.347	38.376	6.434	1.00	16.29	CPS3
ATOM	2727	C	ALA	111	53.819	39.758	8.469	1.00	17.67	CPS3
ATOM	2728	O	ALA	111	53.404	40.903	8.312	1.00	18.51	CPS3
ATOM	2729	N	ALA	112	54.672	39.424	9.428	1.00	16.56	CPS3
ATOM	2730	CA	ALA	112	55.181	40.433	10.342	1.00	15.86	CPS3
ATOM	2731	CB	ALA	112	54.203	40.636	11.489	1.00	15.01	CPS3
ATOM	2732	C	ALA	112	56.533	40.033	10.896	1.00	17.34	CPS3
ATOM	2733	O	ALA	112	56.885	38.856	10.913	1.00	16.61	CPS3
ATOM	2734	N	GLN	113	57.294	41.021	11.352	1.00	16.50	CPS3
ATOM	2735	CA	GLN	113	58.591	40.732	11.952	1.00	18.53	CPS3

FIG. 1A-48

ATOM	2736	CB	GLN	113	59.735	40.962	10.956	1.00	18.24	CPS3
ATOM	2737	CG	GLN	113	59.926	42.406	10.544	1.00	22.84	CPS3
ATOM	2738	CD	GLN	113	61.095	42.611	9.578	1.00	26.07	CPS3
ATOM	2739	OE1	GLN	113	61.504	43.738	9.326	1.00	28.00	CPS3
ATOM	2740	NE2	GLN	113	61.624	41.521	9.033	1.00	28.26	CPS3
ATOM	2741	C	GLN	113	58.724	41.667	13.144	1.00	16.72	CPS3
ATOM	2742	O	GLN	113	58.108	42.728	13.182	1.00	16.09	CPS3
ATOM	2743	N	VAL	114	59.513	41.252	14.124	1.00	17.10	CPS3
ATOM	2744	CA	VAL	114	59.707	42.051	15.329	1.00	17.04	CPS3
ATOM	2745	CB	VAL	114	58.882	41.484	16.538	1.00	17.59	CPS3
ATOM	2746	CG1	VAL	114	59.307	42.160	17.853	1.00	17.11	CPS3
ATOM	2747	CG2	VAL	114	57.392	41.703	16.320	1.00	16.91	CPS3
ATOM	2748	C	VAL	114	61.173	41.971	15.710	1.00	18.24	CPS3
ATOM	2749	O	VAL	114	61.826	40.948	15.493	1.00	16.19	CPS3
ATOM	2750	N	VAL	115	61.691	43.068	16.251	1.00	18.16	CPS3
ATOM	2751	CA	VAL	115	63.053	43.072	16.763	1.00	19.36	CPS3
ATOM	2752	CB	VAL	115	64.021	43.925	15.920	1.00	20.69	CPS3
ATOM	2753	CG1	VAL	115	65.394	44.014	16.637	1.00	20.85	CPS3
ATOM	2754	CG2	VAL	115	64.184	43.305	14.529	1.00	18.29	CPS3
ATOM	2755	C	VAL	115	62.916	43.691	18.148	1.00	20.16	CPS3
ATOM	2756	O	VAL	115	62.268	44.728	18.309	1.00	21.78	CPS3
ATOM	2757	N	ILE	116	63.463	43.018	19.152	1.00	20.33	CPS3
ATOM	2758	CA	ILE	116	63.438	43.527	20.517	1.00	21.08	CPS3
ATOM	2759	CB	ILE	116	62.911	42.491	21.517	1.00	21.66	CPS3
ATOM	2760	CG2	ILE	116	63.081	43.042	22.960	1.00	21.13	CPS3
ATOM	2761	CG1	ILE	116	61.439	42.174	21.215	1.00	21.09	CPS3
ATOM	2762	CD1	ILE	116	60.806	41.091	22.118	1.00	19.60	CPS3
ATOM	2763	C	ILE	116	64.881	43.835	20.885	1.00	24.39	CPS3
ATOM	2764	O	ILE	116	65.764	42.993	20.697	1.00	22.81	CPS3
ATOM	2765	N	GLU	117	65.131	45.041	21.381	1.00	26.58	CPS3
ATOM	2766	CA	GLU	117	66.487	45.410	21.767	1.00	31.31	CPS3
ATOM	2767	CB	GLU	117	66.824	46.834	21.346	1.00	32.50	CPS3
ATOM	2768	CG	GLU	117	66.641	47.178	19.901	1.00	37.84	CPS3
ATOM	2769	CD	GLU	117	67.052	48.616	19.638	1.00	40.98	CPS3
ATOM	2770	OE1	GLU	117	68.271	48.872	19.516	1.00	42.89	CPS3
ATOM	2771	OE2	GLU	117	66.160	49.491	19.578	1.00	43.15	CPS3
ATOM	2772	C	GLU	117	66.653	45.367	23.275	1.00	33.73	CPS3
ATOM	2773	O	GLU	117	65.679	45.454	24.026	1.00	33.05	CPS3
ATOM	2774	N	ARG	118	67.904	45.244	23.708	1.00	37.38	CPS3
ATOM	2775	CA	ARG	118	68.224	45.267	25.124	1.00	41.10	CPS3
ATOM	2776	CB	ARG	118	69.512	44.496	25.407	1.00	42.40	CPS3
ATOM	2777	CG	ARG	118	69.311	43.126	26.025	1.00	44.67	CPS3
ATOM	2778	CD	ARG	118	70.649	42.566	26.483	1.00	45.83	CPS3
ATOM	2779	NE	ARG	118	71.614	42.542	25.389	1.00	47.03	CPS3
ATOM	2780	CZ	ARG	118	71.609	41.652	24.402	1.00	47.03	CPS3
ATOM	2781	NH1	ARG	118	70.690	40.694	24.367	1.00	46.54	CPS3
ATOM	2782	NH2	ARG	118	72.520	41.729	23.446	1.00	46.88	CPS3
ATOM	2783	C	ARG	118	68.452	46.744	25.399	1.00	42.76	CPS3
ATOM	2784	O	ARG	118	69.227	47.392	24.697	1.00	44.45	CPS3
ATOM	2785	N	LEU	119	67.765	47.289	26.392	1.00	45.54	CPS3
ATOM	2786	CA	LEU	119	67.928	48.699	26.722	1.00	47.93	CPS3
ATOM	2787	CB	LEU	119	66.563	49.328	27.014	1.00	48.16	CPS3
ATOM	2788	CG	LEU	119	65.944	50.257	25.963	1.00	47.88	CPS3
ATOM	2789	CD1	LEU	119	66.182	49.739	24.548	1.00	47.81	CPS3
ATOM	2790	CD2	LEU	119	64.460	50.385	26.260	1.00	47.26	CPS3
ATOM	2791	C	LEU	119	68.845	48.862	27.928	1.00	49.49	CPS3
ATOM	2792	OT1	LEU	119	70.001	49.296	27.728	1.00	50.38	CPS3

FIG. 1A-49

ATOM	2793	OT2	LEU	119	68.399	48.537	29.052	1.00	51.04	CPS3
ATOM	2794	C	GLY	0	33.524	21.933	24.405	1.00	41.93	CPS4
ATOM	2795	O	GLY	0	33.109	21.427	23.356	1.00	43.93	CPS4
ATOM	2796	N	GLY	0	35.967	22.519	24.212	1.00	43.67	CPS4
ATOM	2797	CA	GLY	0	34.574	23.033	24.374	1.00	42.80	CPS4
ATOM	2798	N	GLY	1	33.089	21.565	25.607	1.00	38.91	CPS4
ATOM	2799	CA	GLY	1	32.082	20.530	25.746	1.00	34.29	CPS4
ATOM	2800	C	GLY	1	30.697	21.104	25.995	1.00	31.42	CPS4
ATOM	2801	O	GLY	1	29.713	20.369	26.051	1.00	30.75	CPS4
ATOM	2802	N	ILE	2	30.618	22.419	26.172	1.00	28.92	CPS4
ATOM	2803	CA	ILE	2	29.328	23.068	26.405	1.00	26.32	CPS4
ATOM	2804	CB	ILE	2	29.309	23.809	27.765	1.00	26.73	CPS4
ATOM	2805	CG2	ILE	2	28.044	24.683	27.891	1.00	24.71	CPS4
ATOM	2806	CG1	ILE	2	29.358	22.779	28.896	1.00	27.21	CPS4
ATOM	2807	CD1	ILE	2	29.417	23.387	30.265	1.00	28.66	CPS4
ATOM	2808	C	ILE	2	29.028	24.043	25.277	1.00	25.17	CPS4
ATOM	2809	O	ILE	2	29.861	24.874	24.922	1.00	24.41	CPS4
ATOM	2810	N	TYR	3	27.839	23.910	24.703	1.00	24.67	CPS4
ATOM	2811	CA	TYR	3	27.389	24.765	23.606	1.00	24.61	CPS4
ATOM	2812	CB	TYR	3	26.260	24.071	22.850	1.00	27.01	CPS4
ATOM	2813	CG	TYR	3	25.726	24.865	21.681	1.00	29.25	CPS4
ATOM	2814	CD1	TYR	3	26.385	24.861	20.452	1.00	31.33	CPS4
ATOM	2815	CE1	TYR	3	25.916	25.616	19.379	1.00	33.16	CPS4
ATOM	2816	CD2	TYR	3	24.579	25.645	21.811	1.00	31.21	CPS4
ATOM	2817	CE2	TYR	3	24.101	26.409	20.740	1.00	32.57	CPS4
ATOM	2818	CZ	TYR	3	24.776	26.388	19.530	1.00	34.44	CPS4
ATOM	2819	OH	TYR	3	24.328	27.148	18.473	1.00	36.34	CPS4
ATOM	2820	C	TYR	3	26.881	26.103	24.151	1.00	23.47	CPS4
ATOM	2821	O	TYR	3	27.167	27.175	23.609	1.00	22.30	CPS4
ATOM	2822	N	GLY	4	26.111	26.036	25.226	1.00	21.50	CPS4
ATOM	2823	CA	GLY	4	25.597	27.262	25.802	1.00	20.66	CPS4
ATOM	2824	C	GLY	4	24.775	26.974	27.036	1.00	18.15	CPS4
ATOM	2825	O	GLY	4	24.397	25.824	27.275	1.00	17.40	CPS4
ATOM	2826	N	ILE	5	24.519	28.019	27.827	1.00	17.22	CPS4
ATOM	2827	CA	ILE	5	23.725	27.874	29.039	1.00	16.89	CPS4
ATOM	2828	CB	ILE	5	24.585	27.961	30.311	1.00	17.48	CPS4
ATOM	2829	CG2	ILE	5	25.700	26.921	30.241	1.00	16.93	CPS4
ATOM	2830	CG1	ILE	5	25.166	29.374	30.472	1.00	18.44	CPS4
ATOM	2831	CD1	ILE	5	26.002	29.560	31.716	1.00	17.67	CPS4
ATOM	2832	C	ILE	5	22.673	28.972	29.079	1.00	16.76	CPS4
ATOM	2833	O	ILE	5	22.831	30.024	28.457	1.00	17.03	CPS4
ATOM	2834	N	GLY	6	21.601	28.723	29.816	1.00	16.72	CPS4
ATOM	2835	CA	GLY	6	20.537	29.702	29.894	1.00	17.09	CPS4
ATOM	2836	C	GLY	6	19.874	29.687	31.246	1.00	17.29	CPS4
ATOM	2837	O	GLY	6	19.730	28.638	31.869	1.00	17.78	CPS4
ATOM	2838	N	LEU	7	19.485	30.874	31.703	1.00	16.88	CPS4
ATOM	2839	CA	LEU	7	18.825	31.033	32.990	1.00	17.08	CPS4
ATOM	2840	CB	LEU	7	19.803	31.622	34.006	1.00	18.18	CPS4
ATOM	2841	CG	LEU	7	19.251	31.984	35.389	1.00	18.23	CPS4
ATOM	2842	CD1	LEU	7	18.988	30.707	36.200	1.00	17.58	CPS4
ATOM	2843	CD2	LEU	7	20.282	32.875	36.126	1.00	17.74	CPS4
ATOM	2844	C	LEU	7	17.660	31.998	32.817	1.00	18.06	CPS4
ATOM	2845	O	LEU	7	17.775	32.976	32.082	1.00	18.10	CPS4
ATOM	2846	N	ASP	8	16.539	31.712	33.471	1.00	18.02	CPS4
ATOM	2847	CA	ASP	8	15.394	32.612	33.413	1.00	18.03	CPS4
ATOM	2848	CB	ASP	8	14.426	32.202	32.305	1.00	20.37	CPS4
ATOM	2849	CG	ASP	8	13.195	33.108	32.250	1.00	22.41	CPS4

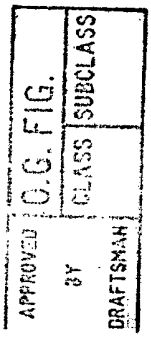
FIG. 1A-50

ATOM	2850	OD1	ASP	8	12.194	32.814	32.922	1.00	25.67	CPS4
ATOM	2851	OD2	ASP	8	13.245	34.131	31.551	1.00	24.39	CPS4
ATOM	2852	C	ASP	8	14.645	32.619	34.732	1.00	19.46	CPS4
ATOM	2853	O	ASP	8	14.490	31.574	35.363	1.00	17.36	CPS4
ATOM	2854	N	ILE	9	14.239	33.806	35.183	1.00	18.34	CPS4
ATOM	2855	CA	ILE	9	13.420	33.898	36.376	1.00	19.60	CPS4
ATOM	2856	CB	ILE	9	14.086	34.711	37.519	1.00	19.76	CPS4
ATOM	2857	CG2	ILE	9	13.133	34.805	38.700	1.00	21.48	CPS4
ATOM	2858	CG1	ILE	9	15.366	34.012	37.982	1.00	20.86	CPS4
ATOM	2859	CD1	ILE	9	16.146	34.790	39.050	1.00	22.16	CPS4
ATOM	2860	C	ILE	9	12.171	34.623	35.878	1.00	20.38	CPS4
ATOM	2861	O	ILE	9	12.277	35.629	35.167	1.00	20.64	CPS4
ATOM	2862	N	THR	10	10.996	34.086	36.205	1.00	19.99	CPS4
ATOM	2863	CA	THR	10	9.749	34.700	35.781	1.00	20.69	CPS4
ATOM	2864	CB	THR	10	8.999	33.803	34.777	1.00	21.55	CPS4
ATOM	2865	OG1	THR	10	9.775	33.679	33.572	1.00	23.30	CPS4
ATOM	2866	CG2	THR	10	7.639	34.414	34.433	1.00	23.59	CPS4
ATOM	2867	C	THR	10	8.833	34.990	36.970	1.00	20.24	CPS4
ATOM	2868	O	THR	10	8.677	34.166	37.865	1.00	18.97	CPS4
ATOM	2869	N	GLU	11	8.233	36.173	36.971	1.00	21.51	CPS4
ATOM	2870	CA	GLU	11	7.321	36.560	38.045	1.00	23.43	CPS4
ATOM	2871	CB	GLU	11	7.180	38.085	38.070	1.00	26.54	CPS4
ATOM	2872	CG	GLU	11	6.189	38.601	39.095	1.00	28.77	CPS4
ATOM	2873	CD	GLU	11	6.072	40.116	39.097	1.00	30.52	CPS4
ATOM	2874	OE1	GLU	11	6.416	40.744	38.078	1.00	29.88	CPS4
ATOM	2875	OE2	GLU	11	5.615	40.675	40.118	1.00	33.84	CPS4
ATOM	2876	C	GLU	11	5.959	35.906	37.791	1.00	24.01	CPS4
ATOM	2877	O	GLU	11	5.344	36.137	36.750	1.00	23.79	CPS4
ATOM	2878	N	LEU	12	5.482	35.092	38.730	1.00	23.66	CPS4
ATOM	2879	CA	LEU	12	4.191	34.416	38.556	1.00	25.00	CPS4
ATOM	2880	CB	LEU	12	3.804	33.609	39.798	1.00	26.31	CPS4
ATOM	2881	CG	LEU	12	4.621	32.386	40.208	1.00	31.01	CPS4
ATOM	2882	CD1	LEU	12	3.877	31.679	41.347	1.00	31.83	CPS4
ATOM	2883	CD2	LEU	12	4.808	31.435	39.028	1.00	32.20	CPS4
ATOM	2884	C	LEU	12	3.044	35.391	38.253	1.00	24.98	CPS4
ATOM	2885	O	LEU	12	2.196	35.107	37.412	1.00	24.51	CPS4
ATOM	2886	N	ALA	13	3.019	36.524	38.950	1.00	25.40	CPS4
ATOM	2887	CA	ALA	13	1.968	37.527	38.744	1.00	25.67	CPS4
ATOM	2888	CB	ALA	13	2.157	38.691	39.702	1.00	28.52	CPS4
ATOM	2889	C	ALA	13	1.939	38.044	37.314	1.00	26.33	CPS4
ATOM	2890	O	ALA	13	0.871	38.344	36.781	1.00	26.54	CPS4
ATOM	2891	N	ARG	14	3.107	38.152	36.688	1.00	24.68	CPS4
ATOM	2892	CA	ARG	14	3.179	38.644	35.318	1.00	26.32	CPS4
ATOM	2893	CB	ARG	14	4.644	38.886	34.925	1.00	28.73	CPS4
ATOM	2894	CG	ARG	14	4.859	39.331	33.482	1.00	34.36	CPS4
ATOM	2895	CD	ARG	14	6.328	39.142	33.058	1.00	37.57	CPS4
ATOM	2896	NE	ARG	14	6.497	39.219	31.608	1.00	41.82	CPS4
ATOM	2897	CZ	ARG	14	7.529	38.704	30.947	1.00	42.56	CPS4
ATOM	2898	NH1	ARG	14	8.491	38.070	31.603	1.00	43.08	CPS4
ATOM	2899	NH2	ARG	14	7.597	38.817	29.627	1.00	44.77	CPS4
ATOM	2900	C	ARG	14	2.533	37.633	34.370	1.00	25.53	CPS4
ATOM	2901	O	ARG	14	1.783	38.001	33.465	1.00	25.68	CPS4
ATOM	2902	N	ILE	15	2.832	36.357	34.585	1.00	24.70	CPS4
ATOM	2903	CA	ILE	15	2.278	35.284	33.763	1.00	25.07	CPS4
ATOM	2904	CB	ILE	15	2.884	33.920	34.153	1.00	24.95	CPS4
ATOM	2905	CG2	ILE	15	2.169	32.782	33.390	1.00	24.82	CPS4
ATOM	2906	CG1	ILE	15	4.382	33.913	33.849	1.00	24.68	CPS4

FIG. 1A-51

ATOM	2907	CD1	ILE	15	4.714	33.980	32.358	1.00 27.32	CPS4
ATOM	2908	C	ILE	15	0.766	35.200	33.950	1.00 26.73	CPS4
ATOM	2909	O	ILE	15	0.009	34.983	32.993	1.00 25.85	CPS4
ATOM	2910	N	ALA	16	0.324	35.352	35.193	1.00 26.46	CPS4
ATOM	2911	CA	ALA	16	-1.104	35.273	35.469	1.00 27.92	CPS4
ATOM	2912	CB	ALA	16	-1.355	35.318	36.975	1.00 28.33	CPS4
ATOM	2913	C	ALA	16	-1.823	36.423	34.774	1.00 29.55	CPS4
ATOM	2914	O	ALA	16	-2.928	36.252	34.240	1.00 29.47	CPS4
ATOM	2915	N	SER	17	-1.191	37.592	34.772	1.00 29.18	CPS4
ATOM	2916	CA	SER	17	-1.783	38.760	34.136	1.00 31.51	CPS4
ATOM	2917	CB	SER	17	-0.944	40.000	34.429	1.00 33.05	CPS4
ATOM	2918	OG	SER	17	-1.421	41.104	33.672	1.00 39.63	CPS4
ATOM	2919	C	SER	17	-1.922	38.574	32.624	1.00 32.08	CPS4
ATOM	2920	O	SER	17	-2.974	38.874	32.045	1.00 31.35	CPS4
ATOM	2921	N	MET	18	-0.871	38.078	31.982	1.00 31.52	CPS4
ATOM	2922	CA	MET	18	-0.912	37.868	30.540	1.00 32.75	CPS4
ATOM	2923	CB	MET	18	0.469	37.482	30.008	1.00 34.03	CPS4
ATOM	2924	CG	MET	18	1.504	38.580	30.147	1.00 38.00	CPS4
ATOM	2925	SD	MET	18	3.076	38.170	29.360	1.00 41,64	CPS4
ATOM	2926	CE	MET	18	3.866	37.225	30.666	1.00 38.75	CPS4
ATOM	2927	C	MET	18	-1.917	36.793	30.156	1.00 32.75	CPS4
ATOM	2928	O	MET	18	-2.689	36.971	29.215	1.00 32.74	CPS4
ATOM	2929	N	ALA	19	-1.906	35.686	30.893	1.00 33.01	CPS4
ATOM	2930	CA	ALA	19	-2.801	34.569	30.618	1.00 34.57	CPS4
ATOM	2931	CB	ALA	19	-2.458	33.384	31.515	1.00 34.76	CPS4
ATOM	2932	C	ALA	19	-4.262	34.944	30.793	1.00 36.04	CPS4
ATOM	2933	O	ALA	19	-5.140	34.338	30.176	1.00 36.08	CPS4
ATOM	2934	N	GLY	20	-4.523	35.942	31.630	1.00 36.62	CPS4
ATOM	2935	CA	GLY	20	-5.896	36.360	31.852	1.00 38.42	CPS4
ATOM	2936	C	GLY	20	-6.379	37.392	30.850	1.00 38.57	CPS4
ATOM	2937	O	GLY	20	-7.560	37.437	30.511	1.00 38.87	CPS4
ATOM	2938	N	ARG	21	-5.460	38.210	30.355	1.00 38.64	CPS4
ATOM	2939	CA	ARG	21	-5.813	39.261	29.417	1.00 39.87	CPS4
ATOM	2940	CB	ARG	21	-4.944	40.489	29.695	1.00 42.18	CPS4
ATOM	2941	CG	ARG	21	-4.955	40.913	31.156	1.00 47.12	CPS4
ATOM	2942	CD	ARG	21	-4.162	42.195	31.381	1.00 50.94	CPS4
ATOM	2943	NE	ARG	21	-4.149	42.582	32.792	1.00 55.15	CPS4
ATOM	2944	CZ	ARG	21	-3.691	43.746	33.252	1.00 56.93	CPS4
ATOM	2945	NH1	ARG	21	-3.721	44.005	34.554	1.00 57.41	CPS4
ATOM	2946	NH2	ARG	21	-3.211	44.656	32.412	1.00 57.54	CPS4
ATOM	2947	C	ARG	21	-5.699	38.879	27.942	1.00 39.28	CPS4
ATOM	2948	O	ARG	21	-6.223	39.587	27.080	1.00 39.05	CPS4
ATOM	2949	N	GLN	22	-5.030	37.764	27.655	1.00 37.77	CPS4
ATOM	2950	CA	GLN	22	-4.823	37.311	26.276	1.00 37.67	CPS4
ATOM	2951	CB	GLN	22	-3.325	37.254	25.979	1.00 36.76	CPS4
ATOM	2952	CG	GLN	22	-2.634	38.603	26.038	1.00 40.23	CPS4
ATOM	2953	CD	GLN	22	-1.135	38.490	25.871	1.00 41.78	CPS4
ATOM	2954	OE1	GLN	22	-0.652	37.746	25.018	1.00 43.79	CPS4
ATOM	2955	NE2	GLN	22	-0.389	39.236	26.677	1.00 42.68	CPS4
ATOM	2956	C	GLN	22	-5.441	35.947	25.997	1.00 37.08	CPS4
ATOM	2957	O	GLN	22	-5.004	34.936	26.560	1.00 37.84	CPS4
ATOM	2958	N	LYS	23	-6.431	35.910	25.106	1.00 34.80	CPS4
ATOM	2959	CA	LYS	23	-7.114	34.661	24.781	1.00 34.70	CPS4
ATOM	2960	CB	LYS	23	-8.133	34.862	23.641	1.00 35.14	CPS4
ATOM	2961	CG	LYS	23	-9.497	35.362	24.090	1.00 37.14	CPS4
ATOM	2962	CD	LYS	23	-10.626	34.901	23.159	1.00 37.66	CPS4
ATOM	2963	CE	LYS	23	-10.491	35.444	21.745	1.00 36.38	CPS4

FIG. 1A-52



ATOM	2964	NZ	LYS	23	-11.732	35.177	20.937	1.00 32.97	CPS4
ATOM	2965	C	LYS	23	-6.211	33.491	24.403	1.00 32.65	CPS4
ATOM	2966	O	LYS	23	-6.488	32.356	24.775	1.00 33.18	CPS4
ATOM	2967	N	ARG	24	-5.143	33.754	23.659	1.00 31.45	CPS4
ATOM	2968	CA	ARG	24	-4.265	32.662	23.227	1.00 31.24	CPS4
ATOM	2969	CB	ARG	24	-4.159	32.665	21.691	1.00 32.20	CPS4
ATOM	2970	CG	ARG	24	-5.218	31.798	20.979	1.00 34.37	CPS4
ATOM	2971	CD	ARG	24	-6.636	32.172	21.379	1.00 34.60	CPS4
ATOM	2972	NE	ARG	24	-7.668	31.404	20.672	1.00 34.87	CPS4
ATOM	2973	CZ	ARG	24	-8.339	30.379	21.191	1.00 34.53	CPS4
ATOM	2974	NH1	ARG	24	-8.095	29.976	22.428	1.00 33.25	CPS4
ATOM	2975	NH2	ARG	24	-9.281	29.770	20.478	1.00 35.11	CPS4
ATOM	2976	C	ARG	24	-2.864	32.603	23.832	1.00 29.23	CPS4
ATOM	2977	O	ARG	24	-1.967	31.992	23.259	1.00 28.10	CPS4
ATOM	2978	N	PHE	25	-2.669	33.208	24.995	1.00 27.93	CPS4
ATOM	2979	CA	PHE	25	-1.339	33.186	25.604	1.00 26.76	CPS4
ATOM	2980	CB	PHE	25	-1.339	33.979	26.916	1.00 27.25	CPS4
ATOM	2981	CG	PHE	25	0.016	34.068	27.564	1.00 28.14	CPS4
ATOM	2982	CD1	PHE	25	0.301	33.345	28.716	1.00 29.02	CPS4
ATOM	2983	CD2	PHE	25	1.023	34.837	26.986	1.00 29.76	CPS4
ATOM	2984	CE1	PHE	25	1.576	33.380	29.286	1.00 29.84	CPS4
ATOM	2985	CE2	PHE	25	2.304	34.879	27.547	1.00 31.14	CPS4
ATOM	2986	CZ	PHE	25	2.579	34.146	28.699	1.00 28.80	CPS4
ATOM	2987	C	PHE	25	-0.822	31.763	25.857	1.00 24.98	CPS4
ATOM	2988	O	PHE	25	0.244	31.385	25.364	1.00 25.69	CPS4
ATOM	2989	N	ALA	26	-1.569	30.979	26.627	1.00 23.55	CPS4
ATOM	2990	CA	ALA	26	-1.158	29.609	26.932	1.00 23.50	CPS4
ATOM	2991	CB	ALA	26	-2.187	28.935	27.812	1.00 23.29	CPS4
ATOM	2992	C	ALA	26	-0.968	28.785	25.668	1.00 23.71	CPS4
ATOM	2993	O	ALA	26	-0.022	27.999	25.567	1.00 22.90	CPS4
ATOM	2994	N	GLU	27	-1.887	28.951	24.719	1.00 23.56	CPS4
ATOM	2995	CA	GLU	27	-1.837	28.211	23.460	1.00 23.91	CPS4
ATOM	2996	CB	GLU	27	-3.114	28.471	22.645	1.00 25.46	CPS4
ATOM	2997	CG	GLU	27	-4.387	27.805	23.184	1.00 28.50	CPS4
ATOM	2998	CD	GLU	27	-4.892	28.403	24.499	1.00 32.43	CPS4
ATOM	2999	OE1	GLU	27	-4.603	29.589	24.774	1.00 31.29	CPS4
ATOM	3000	OE2	GLU	27	-5.589	27.682	25.255	1.00 33.07	CPS4
ATOM	3001	C	GLU	27	-0.610	28.550	22.615	1.00 23.66	CPS4
ATOM	3002	O	GLU	27	-0.152	27.734	21.822	1.00 24.71	CPS4
ATOM	3003	N	ARG	28	-0.081	29.754	22.779	1.00 24.04	CPS4
ATOM	3004	CA	ARG	28	1.094	30.170	22.016	1.00 25.19	CPS4
ATOM	3005	CB	ARG	28	1.191	31.696	22.047	1.00 28.07	CPS4
ATOM	3006	CG	ARG	28	1.800	32.351	20.829	1.00 33.41	CPS4
ATOM	3007	CD	ARG	28	0.994	33.602	20.446	1.00 34.25	CPS4
ATOM	3008	NE	ARG	28	0.767	34.484	21.592	1.00 35.45	CPS4
ATOM	3009	CZ	ARG	28	-0.389	35.097	21.853	1.00 37.30	CPS4
ATOM	3010	NH1	ARG	28	-1.433	34.929	21.050	1.00 35.32	CPS4
ATOM	3011	NH2	ARG	28	-0.506	35.871	22.928	1.00 37.39	CPS4
ATOM	3012	C	ARG	28	2.355	29.564	22.634	1.00 24.51	CPS4
ATOM	3013	O	ARG	28	3.295	29.188	21.933	1.00 23.41	CPS4
ATOM	3014	N	ILE	29	2.348	29.459	23.956	1.00 22.84	CPS4
ATOM	3015	CA	ILE	29	3.498	28.959	24.707	1.00 23.13	CPS4
ATOM	3016	CB	ILE	29	3.462	29.482	26.175	1.00 24.30	CPS4
ATOM	3017	CG2	ILE	29	4.666	28.961	26.957	1.00 24.45	CPS4
ATOM	3018	CG1	ILE	29	3.390	31.014	26.192	1.00 25.98	CPS4
ATOM	3019	CD1	ILE	29	4.519	31.704	25.507	1.00 27.67	CPS4
ATOM	3020	C	ILE	29	3.628	27.450	24.787	1.00 22.56	CPS4

FIG. 1A-53

ATOM	3021	O	ILE	29	4.739	26.914	24.700	1.00 22.11	CPS4
ATOM	3022	N	LEU	30	2.492	26.774	24.952	1.00 20.94	CPS4
ATOM	3023	CA	LEU	30	2.456	25.334	25.150	1.00 20.47	CPS4
ATOM	3024	CB	LEU	30	1.447	25.009	26.264	1.00 20.33	CPS4
ATOM	3025	CG	LEU	30	1.660	25.741	27.600	1.00 23.00	CPS4
ATOM	3026	CD1	LEU	30	0.511	25.425	28.561	1.00 23.25	CPS4
ATOM	3027	CD2	LEU	30	2.999	25.331	28.199	1.00 20.84	CPS4
ATOM	3028	C	LEU	30	2.120	24.493	23.936	1.00 21.35	CPS4
ATOM	3029	O	LEU	30	1.279	24.870	23.127	1.00 22.16	CPS4
ATOM	3030	N	THR	31	2.781	23.344	23.821	1.00 21.39	CPS4
ATOM	3031	CA	THR	31	2.505	22.428	22.727	1.00 22.79	CPS4
ATOM	3032	CB	THR	31	3.594	21.347	22.587	1.00 23.24	CPS4
ATOM	3033	OG1	THR	31	3.631	20.550	23.778	1.00 24.29	CPS4
ATOM	3034	CG2	THR	31	4.960	21.996	22.356	1.00 24.52	CPS4
ATOM	3035	C	THR	31	1.186	21.736	23.052	1.00 25.13	CPS4
ATOM	3036	O	THR	31	0.646	21.868	24.158	1.00 24.76	CPS4
ATOM	3037	N	ARG	32	0.672	20.974	22.096	1.00 27.56	CPS4
ATOM	3038	CA	ARG	32	-0.594	20.289	22.298	1.00 30.79	CPS4
ATOM	3039	CB	ARG	32	-0.951	19.489	21.041	1.00 33.62	CPS4
ATOM	3040	CG	ARG	32	-2.328	19.807	20.476	1.00 38.29	CPS4
ATOM	3041	CD	ARG	32	-3.419	18.876	21.014	1.00 42.11	CPS4
ATOM	3042	NE	ARG	32	-4.044	19.329	22.259	1.00 45.08	CPS4
ATOM	3043	CZ	ARG	32	-4.676	20.491	22.409	1.00 46.06	CPS4
ATOM	3044	NH1	ARG	32	-4.774	21.348	21.393	1.00 45.64	CPS4
ATOM	3045	NH2	ARG	32	-5.224	20.792	23.577	1.00 45.73	CPS4
ATOM	3046	C	ARG	32	-0.577	19.384	23.524	1.00 30.10	CPS4
ATOM	3047	O	ARG	32	-1.527	19.388	24.310	1.00 30.78	CPS4
ATOM	3048	N	SER	33	0.499	18.620	23.699	1.00 30.30	CPS4
ATOM	3049	CA	SER	33	0.615	17.722	24.850	1.00 31.44	CPS4
ATOM	3050	CB	SER	33	1.853	16.833	24.715	1.00 32.43	CPS4
ATOM	3051	OG	SER	33	1.709	15.944	23.620	1.00 37.42	CPS4
ATOM	3052	C	SER	33	0.684	18.489	26.168	1.00 30.59	CPS4
ATOM	3053	O	SER	33	0.054	18.108	27.153	1.00 31.00	CPS4
ATOM	3054	N	GLU	34	1.464	19.564	26.191	1.00 28.83	CPS4
ATOM	3055	CA	GLU	34	1.589	20.370	27.400	1.00 27.36	CPS4
ATOM	3056	CB	GLU	34	2.621	21.487	27.192	1.00 26.46	CPS4
ATOM	3057	CG	GLU	34	4.048	20.963	27.099	1.00 24.49	CPS4
ATOM	3058	CD	GLU	34	5.074	22.029	26.712	1.00 24.80	CPS4
ATOM	3059	OE1	GLU	34	6.223	21.934	27.196	1.00 23.27	CPS4
ATOM	3060	OE2	GLU	34	4.748	22.943	25.920	1.00 23.10	CPS4
ATOM	3061	C	GLU	34	0.232	20.962	27.757	1.00 27.85	CPS4
ATOM	3062	O	GLU	34	-0.138	21.028	28.928	1.00 27.48	CPS4
ATOM	3063	N	LEU	35	-0.513	21.392	26.742	1.00 28.18	CPS4
ATOM	3064	CA	LEU	35	-1.840	21.960	26.968	1.00 29.32	CPS4
ATOM	3065	CB	LEU	35	-2.428	22.478	25.657	1.00 27.71	CPS4
ATOM	3066	CG	LEU	35	-1.986	23.882	25.261	1.00 28.10	CPS4
ATOM	3067	CD1	LEU	35	-2.379	24.130	23.810	1.00 28.81	CPS4
ATOM	3068	CD2	LEU	35	-2.629	24.928	26.202	1.00 25.30	CPS4
ATOM	3069	C	LEU	35	-2.782	20.931	27.572	1.00 30.93	CPS4
ATOM	3070	O	LEU	35	-3.617	21.263	28.417	1.00 31.38	CPS4
ATOM	3071	N	ASP	36	-2.659	19.681	27.135	1.00 33.94	CPS4
ATOM	3072	CA	ASP	36	-3.513	18.632	27.673	1.00 35.97	CPS4
ATOM	3073	CB	ASP	36	-3.206	17.274	27.025	1.00 37.70	CPS4
ATOM	3074	CG	ASP	36	-3.763	17.156	25.612	1.00 39.64	CPS4
ATOM	3075	OD1	ASP	36	-4.838	17.727	25.332	1.00 41.16	CPS4
ATOM	3076	OD2	ASP	36	-3.134	16.475	24.778	1.00 42.22	CPS4
ATOM	3077	C	ASP	36	-3.306	18.560	29.182	1.00 36.01	CPS4

FIG. 1A-54

ATOM	3078	O	ASP	36	-4.269	18.440	29.933	1.00 36.88	CPS4
ATOM	3079	N	GLN	37	-2.054	18.645	29.626	1.00 35.23	CPS4
ATOM	3080	CA	GLN	37	-1.750	18.612	31.057	1.00 34.91	CPS4
ATOM	3081	CB	GLN	37	-0.238	18.552	31.278	1.00 36.27	CPS4
ATOM	3082	CG	GLN	37	0.417	17.271	30.798	1.00 40.16	CPS4
ATOM	3083	CD	GLN	37	1.925	17.394	30.676	1.00 41.54	CPS4
ATOM	3084	OE1	GLN	37	2.436	18.146	29.845	1.00 42.68	CPS4
ATOM	3085	NE2	GLN	37	2.647	16.656	31.509	1.00 43.46	CPS4
ATOM	3086	C	GLN	37	-2.302	19.869	31.722	1.00 33.96	CPS4
ATOM	3087	O	GLN	37	-2.985	19.810	32.743	1.00 33.94	CPS4
ATOM	3088	N	TYR	38	-1.990	21.009	31.120	1.00 32.47	CPS4
ATOM	3089	CA	TYR	38	-2.422	22.315	31.601	1.00 31.95	CPS4
ATOM	3090	CB	TYR	38	-1.938	23.378	30.617	1.00 30.34	CPS4
ATOM	3091	CG	TYR	38	-2.442	24.776	30.869	1.00 29.96	CPS4
ATOM	3092	CD1	TYR	38	-3.488	25.308	30.110	1.00 30.42	CPS4
ATOM	3093	CE1	TYR	38	-3.905	26.618	30.287	1.00 30.73	CPS4
ATOM	3094	CD2	TYR	38	-1.836	25.593	31.821	1.00 28.80	CPS4
ATOM	3095	CE2	TYR	38	-2.248	26.906	32.005	1.00 29.56	CPS4
ATOM	3096	CZ	TYR	38	-3.278	27.411	31.238	1.00 31.46	CPS4
ATOM	3097	OH	TYR	38	-3.689	28.710	31.428	1.00 32.91	CPS4
ATOM	3098	C	TYR	38	-3.936	22.438	31.803	1.00 32.87	CPS4
ATOM	3099	O	TYR	38	-4.388	22.888	32.854	1.00 31.90	CPS4
ATOM	3100	N	TYR	39	-4.716	22.040	30.801	1.00 34.25	CPS4
ATOM	3101	CA	TYR	39	-6.167	22.151	30.905	1.00 36.14	CPS4
ATOM	3102	CB	TYR	39	-6.842	21.687	29.605	1.00 36.53	CPS4
ATOM	3103	CG	TYR	39	-6.618	22.577	28.390	1.00 36.61	CPS4
ATOM	3104	CD1	TYR	39	-6.608	23.970	28.504	1.00 36.59	CPS4
ATOM	3105	CE1	TYR	39	-6.471	24.791	27.378	1.00 37.06	CPS4
ATOM	3106	CD2	TYR	39	-6.483	22.021	27.115	1.00 36.55	CPS4
ATOM	3107	CE2	TYR	39	-6.347	22.830	25.980	1.00 37.48	CPS4
ATOM	3108	CZ	TYR	39	-6.343	24.213	26.118	1.00 37.69	CPS4
ATOM	3109	OH	TYR	39	-6.224	25.011	24.998	1.00 37.54	CPS4
ATOM	3110	C	TYR	39	-6.734	21.354	32.080	1.00 37.42	CPS4
ATOM	3111	O	TYR	39	-7.809	21.667	32.584	1.00 38.66	CPS4
ATOM	3112	N	GLU	40	-6.010	20.334	32.524	1.00 39.15	CPS4
ATOM	3113	CA	GLU	40	-6.476	19.491	33.622	1.00 41.54	CPS4
ATOM	3114	CB	GLU	40	-5.862	18.094	33.502	1.00 43.99	CPS4
ATOM	3115	CG	GLU	40	-6.257	17.341	32.235	1.00 48.54	CPS4
ATOM	3116	CD	GLU	40	-7.761	17.149	32.111	1.00 50.97	CPS4
ATOM	3117	OE1	GLU	40	-8.377	16.647	33.076	1.00 53.41	CPS4
ATOM	3118	OE2	GLU	40	-8.329	17.495	31.050	1.00 52.53	CPS4
ATOM	3119	C	GLU	40	-6.181	20.035	35.009	1.00 41.32	CPS4
ATOM	3120	O	GLU	40	-6.687	19.516	36.006	1.00 41.95	CPS4
ATOM	3121	N	LEU	41	-5.374	21.085	35.075	1.00 40.03	CPS4
ATOM	3122	CA	LEU	41	-4.988	21.666	36.353	1.00 38.83	CPS4
ATOM	3123	CB	LEU	41	-3.589	22.283	36.230	1.00 37.58	CPS4
ATOM	3124	CG	LEU	41	-2.457	21.303	35.908	1.00 36.93	CPS4
ATOM	3125	CD1	LEU	41	-1.171	22.070	35.673	1.00 36.17	CPS4
ATOM	3126	CD2	LEU	41	-2.291	20.309	37.050	1.00 36.43	CPS4
ATOM	3127	C	LEU	41	-5.939	22.709	36.916	1.00 38.96	CPS4
ATOM	3128	O	LEU	41	-6.744	23.295	36.197	1.00 38.34	CPS4
ATOM	3129	N	SER	42	-5.830	22.936	38.220	1.00 39.70	CPS4
ATOM	3130	CA	SER	42	-6.645	23.937	38.890	1.00 41.21	CPS4
ATOM	3131	CB	SER	42	-6.456	23.849	40.408	1.00 41.87	CPS4
ATOM	3132	OG	SER	42	-5.119	24.152	40.781	1.00 40.52	CPS4
ATOM	3133	C	SER	42	-6.182	25.305	38.399	1.00 42.49	CPS4
ATOM	3134	O	SER	42	-5.134	25.424	37.766	1.00 42.26	CPS4

FIG. 1A-55

ATOM	3135	N	GLU	43	-6.955	26.338	38.703	1.00 42.87	CPS4
ATOM	3136	CA	GLU	43	-6.616	27.687	38.286	1.00 44.09	CPS4
ATOM	3137	CB	GLU	43	-7.686	28.651	38.803	1.00 46.92	CPS4
ATOM	3138	CG	GLU	43	-7.721	30.000	38.115	1.00 51.91	CPS4
ATOM	3139	CD	GLU	43	-6.722	30.982	38.687	1.00 55.38	CPS4
ATOM	3140	OE1	GLU	43	-6.747	31.203	39.920	1.00 57.45	CPS4
ATOM	3141	OE2	GLU	43	-5.920	31.543	37.905	1.00 57.72	CPS4
ATOM	3142	C	GLU	43	-5.226	28.088	38.802	1.00 43.04	CPS4
ATOM	3143	O	GLU	43	-4.404	28.633	38.058	1.00 42.48	CPS4
ATOM	3144	N	LYS	44	-4.965	27.805	40.074	1.00 41.59	CPS4
ATOM	3145	CA	LYS	44	-3.684	28.136	40.690	1.00 40.46	CPS4
ATOM	3146	CB	LYS	44	-3.758	27.910	42.201	1.00 42.16	CPS4
ATOM	3147	CG	LYS	44	-2.528	28.378	42.960	1.00 44.29	CPS4
ATOM	3148	CD	LYS	44	-2.684	28.137	44.457	1.00 47.29	CPS4
ATOM	3149	CE	LYS	44	-1.439	28.574	45.218	1.00 48.62	CPS4
ATOM	3150	NZ	LYS	44	-1.554	28.319	46.683	1.00 50.30	CPS4
ATOM	3151	C	LYS	44	-2.537	27.311	40.107	1.00 38.58	CPS4
ATOM	3152	O	LYS	44	-1.466	27.845	39.806	1.00 37.53	CPS4
ATOM	3153	N	ARG	45	-2.764	26.010	39.957	1.00 35.62	CPS4
ATOM	3154	CA	ARG	45	-1.755	25.115	39.406	1.00 34.29	CPS4
ATOM	3155	CB	ARG	45	-2.205	23.663	39.575	1.00 36.05	CPS4
ATOM	3156	CG	ARG	45	-2.054	23.119	41.002	1.00 39.56	CPS4
ATOM	3157	CD	ARG	45	-0.605	22.768	41.301	1.00 42.27	CPS4
ATOM	3158	NE	ARG	45	-0.090	21.793	40.341	1.00 45.82	CPS4
ATOM	3159	CZ	ARG	45	1.003	21.973	39.600	1.00 48.25	CPS4
ATOM	3160	NH1	ARG	45	1.711	23.093	39.707	1.00 47.45	CPS4
ATOM	3161	NH2	ARG	45	1.381	21.037	38.733	1.00 48.96	CPS4
ATOM	3162	C	ARG	45	-1.491	25.422	37.926	1.00 32.63	CPS4
ATOM	3163	O	ARG	45	-0.383	25.215	37.425	1.00 30.48	CPS4
ATOM	3164	N	LYS	46	-2.513	25.912	37.232	1.00 30.94	CPS4
ATOM	3165	CA	LYS	46	-2.365	26.265	35.820	1.00 31.41	CPS4
ATOM	3166	CB	LYS	46	-3.672	26.841	35.262	1.00 31.76	CPS4
ATOM	3167	CG	LYS	46	-4.637	25.828	34.661	1.00 32.98	CPS4
ATOM	3168	CD	LYS	46	-5.770	26.574	33.959	1.00 35.55	CPS4
ATOM	3169	CE	LYS	46	-6.597	25.647	33.081	1.00 37.38	CPS4
ATOM	3170	NZ	LYS	46	-7.283	24.614	33.895	1.00 39.63	CPS4
ATOM	3171	C	LYS	46	-1.275	27.326	35.668	1.00 30.10	CPS4
ATOM	3172	O	LYS	46	-0.365	27.197	34.843	1.00 28.86	CPS4
ATOM	3173	N	ASN	47	-1.378	28.388	36.457	1.00 29.05	CPS4
ATOM	3174	CA	ASN	47	-0.393	29.445	36.357	1.00 29.35	CPS4
ATOM	3175	CB	ASN	47	-0.875	30.700	37.081	1.00 32.62	CPS4
ATOM	3176	CG	ASN	47	-1.923	31.471	36.270	1.00 36.22	CPS4
ATOM	3177	OD1	ASN	47	-1.748	31.710	35.065	1.00 37.87	CPS4
ATOM	3178	ND2	ASN	47	-3.008	31.869	36.928	1.00 38.04	CPS4
ATOM	3179	C	ASN	47	0.998	29.033	36.822	1.00 28.34	CPS4
ATOM	3180	O	ASN	47	1.987	29.533	36.291	1.00 26.63	CPS4
ATOM	3181	N	GLU	48	1.085	28.125	37.794	1.00 27.39	CPS4
ATOM	3182	CA	GLU	48	2.398	27.656	38.253	1.00 26.57	CPS4
ATOM	3183	CB	GLU	48	2.256	26.763	39.493	1.00 29.29	CPS4
ATOM	3184	CG	GLU	48	1.753	27.481	40.733	1.00 35.14	CPS4
ATOM	3185	CD	GLU	48	1.467	26.534	41.899	1.00 38.18	CPS4
ATOM	3186	OE1	GLU	48	1.054	27.029	42.970	1.00 39.62	CPS4
ATOM	3187	OE2	GLU	48	1.654	25.301	41.747	1.00 39.49	CPS4
ATOM	3188	C	GLU	48	3.023	26.848	37.114	1.00 24.55	CPS4
ATOM	3189	O	GLU	48	4.198	27.004	36.786	1.00 23.53	CPS4
ATOM	3190	N	PHE	49	2.215	25.984	36.513	1.00 22.65	CPS4
ATOM	3191	CA	PHE	49	2.643	25.136	35.400	1.00 22.71	CPS4

FIG. 1A-56

ATOM	3192	CB	PHE	49	1.474	24.235	34.972	1.00	23.78	CPS4
ATOM	3193	CG	PHE	49	1.796	23.299	33.836	1.00	23.79	CPS4
ATOM	3194	CD1	PHE	49	2.359	22.053	34.084	1.00	25.06	CPS4
ATOM	3195	CD2	PHE	49	1.525	23.660	32.522	1.00	24.25	CPS4
ATOM	3196	CE1	PHE	49	2.645	21.179	33.045	1.00	25.26	CPS4
ATOM	3197	CE2	PHE	49	1.812	22.786	31.464	1.00	25.16	CPS4
ATOM	3198	CZ	PHE	49	2.370	21.546	31.729	1.00	26.61	CPS4
ATOM	3199	C	PHE	49	3.089	25.980	34.201	1.00	22.04	CPS4
ATOM	3200	O	PHE	49	4.158	25.751	33.631	1.00	21.19	CPS4
ATOM	3201	N	LEU	50	2.260	26.945	33.818	1.00	21.02	CPS4
ATOM	3202	CA	LEU	50	2.564	27.807	32.678	1.00	21.41	CPS4
ATOM	3203	CB	LEU	50	1.386	28.749	32.389	1.00	21.73	CPS4
ATOM	3204	CG	LEU	50	1.487	29.682	31.172	1.00	24.05	CPS4
ATOM	3205	CD1	LEU	50	1.697	28.873	29.891	1.00	24.04	CPS4
ATOM	3206	CD2	LEU	50	0.218	30.518	31.075	1.00	23.32	CPS4
ATOM	3207	C	LEU	50	3.832	28.624	32.922	1.00	21.21	CPS4
ATOM	3208	O	LEU	50	4.680	28.724	32.039	1.00	20.96	CPS4
ATOM	3209	N	ALA	51	3.960	29.207	34.114	1.00	19.78	CPS4
ATOM	3210	CA	ALA	51	5.150	30.005	34.432	1.00	19.68	CPS4
ATOM	3211	CB	ALA	51	5.017	30.616	35.830	1.00	20.19	CPS4
ATOM	3212	C	ALA	51	6.417	29.151	34.350	1.00	20.59	CPS4
ATOM	3213	O	ALA	51	7.453	29.598	33.830	1.00	20.05	CPS4
ATOM	3214	N	GLY	52	6.325	27.928	34.865	1.00	20.38	CPS4
ATOM	3215	CA	GLY	52	7.459	27.015	34.840	1.00	20.83	CPS4
ATOM	3216	C	GLY	52	7.861	26.619	33.429	1.00	20.53	CPS4
ATOM	3217	O	GLY	52	9.048	26.587	33.104	1.00	20.29	CPS4
ATOM	3218	N	ARG	53	6.884	26.279	32.593	1.00	21.19	CPS4
ATOM	3219	CA	ARG	53	7.187	25.916	31.207	1.00	21.65	CPS4
ATOM	3220	CB	ARG	53	5.938	25.336	30.532	1.00	23.50	CPS4
ATOM	3221	CG	ARG	53	5.824	23.807	30.654	1.00	26.67	CPS4
ATOM	3222	CD	ARG	53	5.988	23.291	32.077	1.00	31.06	CPS4
ATOM	3223	NE	ARG	53	5.877	21.832	32.121	1.00	35.13	CPS4
ATOM	3224	CZ	ARG	53	6.220	21.082	33.164	1.00	38.06	CPS4
ATOM	3225	NH1	ARG	53	6.702	21.649	34.267	1.00	38.57	CPS4
ATOM	3226	NH2	ARG	53	6.086	19.762	33.105	1.00	39.34	CPS4
ATOM	3227	C	ARG	53	7.710	27.140	30.445	1.00	20.71	CPS4
ATOM	3228	O	ARG	53	8.598	27.030	29.606	1.00	20.01	CPS4
ATOM	3229	N	PHE	54	7.160	28.311	30.740	1.00	20.84	CPS4
ATOM	3230	CA	PHE	54	7.613	29.545	30.090	1.00	19.84	CPS4
ATOM	3231	CB	PHE	54	6.742	30.722	30.558	1.00	19.76	CPS4
ATOM	3232	CG	PHE	54	7.131	32.059	29.966	1.00	22.53	CPS4
ATOM	3233	CD1	PHE	54	7.984	32.922	30.654	1.00	21.19	CPS4
ATOM	3234	CD2	PHE	54	6.638	32.457	28.728	1.00	22.55	CPS4
ATOM	3235	CE1	PHE	54	8.339	34.162	30.115	1.00	22.92	CPS4
ATOM	3236	CE2	PHE	54	6.989	33.701	28.181	1.00	24.30	CPS4
ATOM	3237	CZ	PHE	54	7.846	34.553	28.883	1.00	22.82	CPS4
ATOM	3238	C	PHE	54	9.086	29.791	30.452	1.00	20.51	CPS4
ATOM	3239	O	PHE	54	9.912	30.084	29.583	1.00	19.99	CPS4
ATOM	3240	N	ALA	55	9.419	29.656	31.735	1.00	19.95	CPS4
ATOM	3241	CA	ALA	55	10.798	29.874	32.179	1.00	18.42	CPS4
ATOM	3242	CB	ALA	55	10.885	29.789	33.712	1.00	17.59	CPS4
ATOM	3243	C	ALA	55	11.747	28.867	31.535	1.00	18.74	CPS4
ATOM	3244	O	ALA	55	12.840	29.228	31.097	1.00	17.86	CPS4
ATOM	3245	N	ALA	56	11.329	27.608	31.470	1.00	17.67	CPS4
ATOM	3246	CA	ALA	56	12.173	26.570	30.870	1.00	17.97	CPS4
ATOM	3247	CB	ALA	56	11.519	25.179	31.051	1.00	16.50	CPS4
ATOM	3248	C	ALA	56	12.435	26.845	29.391	1.00	17.61	CPS4

FIG. 1A-57

ATOM	3249	O	ALA	56	13.555	26.672	28.898	1.00 17.56	CPS4
ATOM	3250	N	LYS	57	11.411	27.286	28.669	1.00 17.23	CPS4
ATOM	3251	CA	LYS	57	11.603	27.555	27.249	1.00 17.45	CPS4
ATOM	3252	CB	LYS	57	10.243	27.657	26.535	1.00 17.90	CPS4
ATOM	3253	CG	LYS	57	9.470	26.320	26.585	1.00 17.50	CPS4
ATOM	3254	CD	LYS	57	8.243	26.286	25.673	1.00 19.16	CPS4
ATOM	3255	CE	LYS	57	7.453	24.998	25.915	1.00 20.14	CPS4
ATOM	3256	NZ	LYS	57	6.468	24.688	24.832	1.00 18.82	CPS4
ATOM	3257	C	LYS	57	12.450	28.800	27.033	1.00 18.57	CPS4
ATOM	3258	O	LYS	57	13.282	28.840	26.123	1.00 18.35	CPS4
ATOM	3259	N	GLU	58	12.254	29.815	27.863	1.00 19.33	CPS4
ATOM	3260	CA	GLU	58	13.057	31.018	27.733	1.00 19.47	CPS4
ATOM	3261	CB	GLU	58	12.581	32.104	28.698	1.00 21.46	CPS4
ATOM	3262	CG	GLU	58	11.276	32.786	28.308	1.00 24.96	CPS4
ATOM	3263	CD	GLU	58	11.375	33.576	27.003	1.00 28.39	CPS4
ATOM	3264	OE1	GLU	58	12.482	34.040	26.654	1.00 30.73	CPS4
ATOM	3265	OE2	GLU	58	10.333	33.748	26.333	1.00 31.57	CPS4
ATOM	3266	C	GLU	58	14.504	30.649	28.047	1.00 19.45	CPS4
ATOM	3267	O	GLU	58	15.424	31.075	27.338	1.00 18.48	CPS4
ATOM	3268	N	ALA	59	14.718	29.857	29.097	1.00 17.21	CPS4
ATOM	3269	CA	ALA	59	16.095	29.458	29.434	1.00 16.93	CPS4
ATOM	3270	CB	ALA	59	16.130	28.630	30.730	1.00 16.23	CPS4
ATOM	3271	C	ALA	59	16.704	28.663	28.288	1.00 17.64	CPS4
ATOM	3272	O	ALA	59	17.868	28.871	27.917	1.00 18.71	CPS4
ATOM	3273	N	PHE	60	15.925	27.752	27.708	1.00 17.49	CPS4
ATOM	3274	CA	PHE	60	16.438	26.973	26.590	1.00 17.61	CPS4
ATOM	3275	CB	PHE	60	15.404	25.953	26.093	1.00 17.74	CPS4
ATOM	3276	CG	PHE	60	15.860	25.203	24.869	1.00 19.99	CPS4
ATOM	3277	CD1	PHE	60	16.682	24.085	24.992	1.00 21.60	CPS4
ATOM	3278	CD2	PHE	60	15.565	25.681	23.594	1.00 21.01	CPS4
ATOM	3279	CE1	PHE	60	17.214	23.453	23.863	1.00 21.01	CPS4
ATOM	3280	CE2	PHE	60	16.092	25.059	22.452	1.00 20.43	CPS4
ATOM	3281	CZ	PHE	60	16.922	23.941	22.595	1.00 22.76	CPS4
ATOM	3282	C	PHE	60	16.817	27.894	25.423	1.00 16.99	CPS4
ATOM	3283	O	PHE	60	17.853	27.701	24.792	1.00 18.28	CPS4
ATOM	3284	N	SER	61	15.983	28.894	25.139	1.00 17.64	CPS4
ATOM	3285	CA	SER	61	16.263	29.801	24.026	1.00 17.54	CPS4
ATOM	3286	CB	SER	61	15.069	30.757	23.788	1.00 18.97	CPS4
ATOM	3287	OG	SER	61	15.017	31.816	24.738	1.00 20.70	CPS4
ATOM	3288	C	SER	61	17.554	30.586	24.261	1.00 18.58	CPS4
ATOM	3289	O	SER	61	18.257	30.932	23.312	1.00 19.96	CPS4
ATOM	3290	N	LYS	62	17.873	30.856	25.520	1.00 17.38	CPS4
ATOM	3291	CA	LYS	62	19.095	31.579	25.855	1.00 18.60	CPS4
ATOM	3292	CB	LYS	62	19.021	32.120	27.281	1.00 19.12	CPS4
ATOM	3293	CG	LYS	62	17.939	33.199	27.436	1.00 24.19	CPS4
ATOM	3294	CD	LYS	62	17.990	33.882	28.791	1.00 27.64	CPS4
ATOM	3295	CE	LYS	62	17.112	35.126	28.763	1.00 31.95	CPS4
ATOM	3296	NZ	LYS	62	17.485	36.123	29.784	1.00 34.09	CPS4
ATOM	3297	C	LYS	62	20.309	30.684	25.699	1.00 18.38	CPS4
ATOM	3298	O	LYS	62	21.375	31.133	25.259	1.00 19.22	CPS4
ATOM	3299	N	ALA	63	20.156	29.418	26.070	1.00 17.11	CPS4
ATOM	3300	CA	ALA	63	21.248	28.460	25.934	1.00 17.76	CPS4
ATOM	3301	CB	ALA	63	20.878	27.114	26.619	1.00 16.67	CPS4
ATOM	3302	C	ALA	63	21.497	28.239	24.445	1.00 18.66	CPS4
ATOM	3303	O	ALA	63	22.640	28.126	24.012	1.00 17.98	CPS4
ATOM	3304	N	PHE	64	20.412	28.183	23.672	1.00 18.77	CPS4
ATOM	3305	CA	PHE	64	20.480	27.976	22.220	1.00 19.86	CPS4

FIG. 1A-58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ATOM   3306  CB  PHE  64      19.068  27.758  21.659  1.00 21.49      CPS4
ATOM   3307  CG  PHE  64      19.049  27.258  20.239  1.00 23.19      CPS4
ATOM   3308  CD1 PHE  64      19.603  26.019  19.917  1.00 25.84      CPS4
ATOM   3309  CD2 PHE  64      18.498  28.038  19.223  1.00 24.38      CPS4
ATOM   3310  CE1 PHE  64      19.612  25.558  18.592  1.00 27.01      CPS4
ATOM   3311  CE2 PHE  64      18.495  27.595  17.897  1.00 25.99      CPS4
ATOM   3312  CZ  PHE  64      19.055  26.353  17.578  1.00 25.96      CPS4
ATOM   3313  C   PHE  64      21.142  29.177  21.547  1.00 21.18      CPS4
ATOM   3314  O   PHE  64      21.687  29.057  20.446  1.00 22.00      CPS4
ATOM   3315  N   GLY  65      21.075  30.330  22.214  1.00 20.65      CPS4
ATOM   3316  CA  GLY  65      21.711  31.547  21.735  1.00 21.45      CPS4
ATOM   3317  C   GLY  65      20.914  32.487  20.848  1.00 23.53      CPS4
ATOM   3318  O   GLY  65      21.453  33.483  20.370  1.00 24.12      CPS4
ATOM   3319  N   THR  66      19.635  32.195  20.640  1.00 22.34      CPS4
ATOM   3320  CA  THR  66      18.807  33.016  19.755  1.00 23.68      CPS4
ATOM   3321  CB  THR  66      18.176  32.144  18.667  1.00 25.10      CPS4
ATOM   3322  OG1 THR  66      17.343  31.160  19.296  1.00 25.13      CPS4
ATOM   3323  CG2 THR  66      19.249  31.434  17.845  1.00 26.27      CPS4
ATOM   3324  C   THR  66      17.646  33.737  20.424  1.00 24.40      CPS4
ATOM   3325  O   THR  66      17.172  34.762  19.925  1.00 23.79      CPS4
ATOM   3326  N   GLY  67      17.184  33.199  21.546  1.00 23.11      CPS4
ATOM   3327  CA  GLY  67      16.018  33.766  22.193  1.00 22.95      CPS4
ATOM   3328  C   GLY  67      14.822  33.246  21.391  1.00 23.58      CPS4
ATOM   3329  O   GLY  67      14.997  32.581  20.369  1.00 22.81      CPS4
ATOM   3330  N   ILE  68      13.610  33.540  21.848  1.00 24.83      CPS4
ATOM   3331  CA  ILE  68      12.401  33.107  21.150  1.00 25.43      CPS4
ATOM   3332  CB  ILE  68      11.194  33.083  22.110  1.00 25.71      CPS4
ATOM   3333  CG2 ILE  68       9.899  32.729  21.345  1.00 26.85      CPS4
ATOM   3334  CG1 ILE  68      11.449  32.061  23.222  1.00 24.50      CPS4
ATOM   3335  CD1 ILE  68      11.495  30.626  22.739  1.00 24.17      CPS4
ATOM   3336  C   ILE  68      12.129  34.086  20.007  1.00 27.56      CPS4
ATOM   3337  O   ILE  68      12.150  35.300  20.203  1.00 27.28      CPS4
ATOM   3338  N   GLY  69      11.890  33.559  18.813  1.00 27.53      CPS4
ATOM   3339  CA  GLY  69      11.641  34.434  17.686  1.00 30.15      CPS4
ATOM   3340  C   GLY  69      11.685  33.725  16.353  1.00 30.54      CPS4
ATOM   3341  O   GLY  69      11.274  32.575  16.240  1.00 30.54      CPS4
ATOM   3342  N   ALA  70      12.197  34.416  15.342  1.00 32.70      CPS4
ATOM   3343  CA  ALA  70      12.272  33.860  13.998  1.00 33.34      CPS4
ATOM   3344  CB  ALA  70      12.896  34.886  13.043  1.00 35.40      CPS4
ATOM   3345  C   ALA  70      13.038  32.551  13.917  1.00 33.51      CPS4
ATOM   3346  O   ALA  70      12.695  31.679  13.118  1.00 34.32      CPS4
ATOM   3347  N   GLN  71      14.061  32.398  14.752  1.00 32.10      CPS4
ATOM   3348  CA  GLN  71      14.882  31.192  14.713  1.00 30.79      CPS4
ATOM   3349  CB  GLN  71      16.334  31.545  15.039  1.00 33.45      CPS4
ATOM   3350  CG  GLN  71      16.936  32.597  14.127  1.00 37.57      CPS4
ATOM   3351  CD  GLN  71      18.391  32.873  14.451  1.00 38.92      CPS4
ATOM   3352  OE1 GLN  71      19.258  32.016  14.257  1.00 40.93      CPS4
ATOM   3353  NE2 GLN  71      18.665  34.069  14.961  1.00 40.14      CPS4
ATOM   3354  C   GLN  71      14.443  30.066  15.636  1.00 28.73      CPS4
ATOM   3355  O   GLN  71      14.851  28.923  15.454  1.00 28.34      CPS4
ATOM   3356  N   LEU  72      13.626  30.384  16.633  1.00 26.49      CPS4
ATOM   3357  CA  LEU  72      13.182  29.369  17.575  1.00 24.09      CPS4
ATOM   3358  CB  LEU  72      14.224  29.221  18.690  1.00 24.17      CPS4
ATOM   3359  CG  LEU  72      13.988  28.183  19.791  1.00 23.09      CPS4
ATOM   3360  CD1 LEU  72      14.211  26.785  19.231  1.00 23.74      CPS4
ATOM   3361  CD2 LEU  72      14.948  28.457  20.955  1.00 25.05      CPS4
ATOM   3362  C   LEU  72      11.847  29.777  18.169  1.00 23.32      CPS4
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FIG. 1A-59

ATOM	3363	O	LEU	72	11.699	30.876	18.688	1.00	24.09	CPS4
ATOM	3364	N	SER	73	10.880	28.877	18.084	1.00	22.99	CPS4
ATOM	3365	CA	SER	73	9.542	29.112	18.601	1.00	23.16	CPS4
ATOM	3366	CB	SER	73	8.527	28.653	17.555	1.00	23.80	CPS4
ATOM	3367	OG	SER	73	7.227	28.611	18.093	1.00	29.93	CPS4
ATOM	3368	C	SER	73	9.297	28.339	19.896	1.00	22.31	CPS4
ATOM	3369	O	SER	73	9.976	27.353	20.175	1.00	21.09	CPS4
ATOM	3370	N	PHE	74	8.334	28.803	20.692	1.00	22.33	CPS4
ATOM	3371	CA	PHE	74	7.962	28.093	21.914	1.00	21.01	CPS4
ATOM	3372	CB	PHE	74	6.802	28.801	22.625	1.00	21.02	CPS4
ATOM	3373	CG	PHE	74	7.201	30.032	23.386	1.00	23.04	CPS4
ATOM	3374	CD1	PHE	74	8.018	29.937	24.508	1.00	23.64	CPS4
ATOM	3375	CD2	PHE	74	6.726	31.285	23.003	1.00	22.57	CPS4
ATOM	3376	CE1	PHE	74	8.355	31.074	25.246	1.00	25.06	CPS4
ATOM	3377	CE2	PHE	74	7.057	32.423	23.728	1.00	25.56	CPS4
ATOM	3378	CZ	PHE	74	7.872	32.318	24.854	1.00	24.29	CPS4
ATOM	3379	C	PHE	74	7.470	26.714	21.479	1.00	21.66	CPS4
ATOM	3380	O	PHE	74	7.567	25.744	22.224	1.00	20.92	CPS4
ATOM	3381	N	GLN	75	6.928	26.635	20.266	1.00	20.29	CPS4
ATOM	3382	CA	GLN	75	6.402	25.372	19.760	1.00	21.28	CPS4
ATOM	3383	CB	GLN	75	5.442	25.637	18.595	1.00	22.50	CPS4
ATOM	3384	CG	GLN	75	4.216	26.457	18.996	1.00	22.28	CPS4
ATOM	3385	CD	GLN	75	3.364	25.763	20.048	1.00	22.84	CPS4
ATOM	3386	OE1	GLN	75	2.914	26.384	21.020	1.00	25.78	CPS4
ATOM	3387	NE2	GLN	75	3.133	24.471	19.858	1.00	21.79	CPS4
ATOM	3388	C	GLN	75	7.482	24.374	19.334	1.00	21.34	CPS4
ATOM	3389	O	GLN	75	7.179	23.209	19.072	1.00	22.34	CPS4
ATOM	3390	N	ASP	76	8.732	24.835	19.277	1.00	20.43	CPS4
ATOM	3391	CA	ASP	76	9.872	23.989	18.903	1.00	20.89	CPS4
ATOM	3392	CB	ASP	76	11.006	24.827	18.294	1.00	22.04	CPS4
ATOM	3393	CG	ASP	76	10.672	25.375	16.922	1.00	25.59	CPS4
ATOM	3394	OD1	ASP	76	10.016	24.658	16.149	1.00	28.36	CPS4
ATOM	3395	OD2	ASP	76	11.094	26.513	16.614	1.00	25.63	CPS4
ATOM	3396	C	ASP	76	10.442	23.292	20.132	1.00	20.74	CPS4
ATOM	3397	O	ASP	76	11.380	22.499	20.025	1.00	20.53	CPS4
ATOM	3398	N	ILE	77	9.869	23.586	21.291	1.00	19.74	CPS4
ATOM	3399	CA	ILE	77	10.353	23.033	22.551	1.00	19.49	CPS4
ATOM	3400	CB	ILE	77	10.944	24.160	23.433	1.00	18.31	CPS4
ATOM	3401	CG2	ILE	77	11.700	23.554	24.627	1.00	19.88	CPS4
ATOM	3402	CG1	ILE	77	11.856	25.056	22.584	1.00	19.12	CPS4
ATOM	3403	CD1	ILE	77	12.172	26.401	23.232	1.00	18.75	CPS4
ATOM	3404	C	ILE	77	9.249	22.387	23.356	1.00	20.14	CPS4
ATOM	3405	O	ILE	77	8.162	22.932	23.474	1.00	21.52	CPS4
ATOM	3406	N	GLU	78	9.530	21.233	23.942	1.00	20.14	CPS4
ATOM	3407	CA	GLU	78	8.520	20.590	24.760	1.00	21.03	CPS4
ATOM	3408	CB	GLU	78	7.814	19.483	23.964	1.00	22.66	CPS4
ATOM	3409	CG	GLU	78	6.792	18.707	24.772	1.00	23.61	CPS4
ATOM	3410	CD	GLU	78	5.914	17.815	23.903	1.00	26.69	CPS4
ATOM	3411	OE1	GLU	78	5.039	18.352	23.195	1.00	26.76	CPS4
ATOM	3412	OE2	GLU	78	6.105	16.581	23.922	1.00	27.97	CPS4
ATOM	3413	C	GLU	78	9.153	20.025	26.014	1.00	20.86	CPS4
ATOM	3414	O	GLU	78	10.219	19.411	25.953	1.00	20.47	CPS4
ATOM	3415	N	ILE	79	8.519	20.273	27.158	1.00	20.68	CPS4
ATOM	3416	CA	ILE	79	9.019	19.744	28.420	1.00	21.74	CPS4
ATOM	3417	CB	ILE	79	8.845	20.756	29.598	1.00	24.16	CPS4
ATOM	3418	CG2	ILE	79	9.053	20.044	30.937	1.00	23.26	CPS4
ATOM	3419	CG1	ILE	79	9.868	21.891	29.485	1.00	27.28	CPS4

FIG. 1A-60

ATOM	3420	CD1	ILE	79	9.772	22.726	28.227	1.00 28.49	CPS4
ATOM	3421	C	ILE	79	8.234	18.478	28.748	1.00 22.41	CPS4
ATOM	3422	O	ILE	79	7.001	18.462	28.685	1.00 22.59	CPS4
ATOM	3423	N	ARG	80	8.958	17.417	29.075	1.00 22.76	CPS4
ATOM	3424	CA	ARG	80	8.349	16.151	29.451	1.00 24.99	CPS4
ATOM	3425	CB	ARG	80	8.684	15.081	28.419	1.00 25.33	CPS4
ATOM	3426	CG	ARG	80	8.181	15.426	27.038	1.00 28.31	CPS4
ATOM	3427	CD	ARG	80	8.496	14.332	26.049	1.00 31.70	CPS4
ATOM	3428	NE	ARG	80	7.736	14.538	24.828	1.00 33.61	CPS4
ATOM	3429	CZ	ARG	80	7.701	13.677	23.820	1.00 35.93	CPS4
ATOM	3430	NH1	ARG	80	8.390	12.545	23.893	1.00 34.86	CPS4
ATOM	3431	NH2	ARG	80	6.974	13.952	22.743	1.00 35.80	CPS4
ATOM	3432	C	ARG	80	8.938	15.777	30.802	1.00 26.08	CPS4
ATOM	3433	O	ARG	80	9.892	16.412	31.257	1.00 22.69	CPS4
ATOM	3434	N	LYS	81	8.372	14.760	31.448	1.00 27.41	CPS4
ATOM	3435	CA	LYS	81	8.877	14.334	32.750	1.00 29.89	CPS4
ATOM	3436	CB	LYS	81	7.866	14.652	33.858	1.00 31.74	CPS4
ATOM	3437	CG	LYS	81	7.741	16.134	34.201	1.00 36.20	CPS4
ATOM	3438	CD	LYS	81	6.836	16.335	35.421	1.00 39.03	CPS4
ATOM	3439	CE	LYS	81	6.576	17.813	35.724	1.00 41.06	CPS4
ATOM	3440	NZ	LYS	81	7.812	18.590	36.021	1.00 41.14	CPS4
ATOM	3441	C	LYS	81	9.157	12.844	32.742	1.00 31.20	CPS4
ATOM	3442	O	LYS	81	8.378	12.069	32.185	1.00 30.64	CPS4
ATOM	3443	N	ASP	82	10.270	12.432	33.341	1.00 30.63	CPS4
ATOM	3444	CA	ASP	82	10.567	11.010	33.374	1.00 31.88	CPS4
ATOM	3445	CB	ASP	82	12.073	10.746	33.491	1.00 30.04	CPS4
ATOM	3446	CG	ASP	82	12.670	11.248	34.788	1.00 30.81	CPS4
ATOM	3447	OD1	ASP	82	11.938	11.421	35.789	1.00 31.13	CPS4
ATOM	3448	OD2	ASP	82	13.899	11.447	34.805	1.00 31.19	CPS4
ATOM	3449	C	ASP	82	9.820	10.351	34.523	1.00 32.86	CPS4
ATOM	3450	O	ASP	82	9.037	10.997	35.221	1.00 32.72	CPS4
ATOM	3451	N	GLN	83	10.063	9.059	34.710	1.00 35.26	CPS4
ATOM	3452	CA	GLN	83	9.404	8.292	35.755	1.00 37.75	CPS4
ATOM	3453	CB	GLN	83	9.861	6.827	35.684	1.00 40.68	CPS4
ATOM	3454	CG	GLN	83	11.357	6.615	35.407	1.00 45.63	CPS4
ATOM	3455	CD	GLN	83	11.805	7.096	34.020	1.00 48.44	CPS4
ATOM	3456	OE1	GLN	83	11.016	7.130	33.068	1.00 49.61	CPS4
ATOM	3457	NE2	GLN	83	13.086	7.447	33.901	1.00 50.02	CPS4
ATOM	3458	C	GLN	83	9.607	8.854	37.160	1.00 38.09	CPS4
ATOM	3459	O	GLN	83	8.748	8.688	38.026	1.00 38.46	CPS4
ATOM	3460	N	ASN	84	10.733	9.528	37.386	1.00 37.38	CPS4
ATOM	3461	CA	ASN	84	11.012	10.119	38.692	1.00 36.22	CPS4
ATOM	3462	CB	ASN	84	12.520	10.213	38.931	1.00 37.16	CPS4
ATOM	3463	CG	ASN	84	13.170	8.858	39.110	1.00 37.93	CPS4
ATOM	3464	OD1	ASN	84	12.631	7.984	39.787	1.00 39.18	CPS4
ATOM	3465	ND2	ASN	84	14.343	8.682	38.518	1.00 39.57	CPS4
ATOM	3466	C	ASN	84	10.404	11.512	38.834	1.00 36.01	CPS4
ATOM	3467	O	ASN	84	10.470	12.118	39.903	1.00 37.22	CPS4
ATOM	3468	N	GLY	85	9.817	12.027	37.759	1.00 34.03	CPS4
ATOM	3469	CA	GLY	85	9.226	13.352	37.824	1.00 31.62	CPS4
ATOM	3470	C	GLY	85	10.203	14.446	37.408	1.00 29.19	CPS4
ATOM	3471	O	GLY	85	9.904	15.632	37.517	1.00 28.96	CPS4
ATOM	3472	N	LYS	86	11.377	14.048	36.938	1.00 26.53	CPS4
ATOM	3473	CA	LYS	86	12.394	15.009	36.507	1.00 25.85	CPS4
ATOM	3474	CB	LYS	86	13.775	14.336	36.511	1.00 26.12	CPS4
ATOM	3475	CG	LYS	86	14.913	15.136	35.853	1.00 24.62	CPS4
ATOM	3476	CD	LYS	86	15.358	16.357	36.678	1.00 22.52	CPS4

FIG. 1A-61

ATOM	3477	CE	LYS	86	16.368	17.189	35.880	1.00	23.49	CPS4
ATOM	3478	NZ	LYS	86	17.044	18.252	36.687	1.00	21.98	CPS4
ATOM	3479	C	LYS	86	12.069	15.527	35.105	1.00	25.27	CPS4
ATOM	3480	O	LYS	86	11.868	14.746	34.175	1.00	23.72	CPS4
ATOM	3481	N	PRO	87	11.987	16.859	34.936	1.00	24.18	CPS4
ATOM	3482	CD	PRO	87	12.068	17.970	35.906	1.00	24.38	CPS4
ATOM	3483	CA	PRO	87	11.682	17.351	33.589	1.00	23.07	CPS4
ATOM	3484	CB	PRO	87	11.343	18.825	33.822	1.00	24.68	CPS4
ATOM	3485	CG	PRO	87	12.229	19.189	34.995	1.00	24.14	CPS4
ATOM	3486	C	PRO	87	12.869	17.202	32.658	1.00	22.51	CPS4
ATOM	3487	O	PRO	87	14.028	17.182	33.098	1.00	21.21	CPS4
ATOM	3488	N	TYR	88	12.576	17.094	31.366	1.00	21.14	CPS4
ATOM	3489	CA	TYR	88	13.617	17.009	30.363	1.00	21.50	CPS4
ATOM	3490	CB	TYR	88	14.069	15.563	30.132	1.00	23.25	CPS4
ATOM	3491	CG	TYR	88	13.032	14.648	29.546	1.00	24.04	CPS4
ATOM	3492	CD1	TYR	88	12.953	14.449	28.165	1.00	26.52	CPS4
ATOM	3493	CE1	TYR	88	12.033	13.554	27.622	1.00	27.83	CPS4
ATOM	3494	CD2	TYR	88	12.164	13.941	30.369	1.00	25.98	CPS4
ATOM	3495	CE2	TYR	88	11.241	13.048	29.840	1.00	27.07	CPS4
ATOM	3496	CZ	TYR	88	11.185	12.857	28.467	1.00	28.72	CPS4
ATOM	3497	OH	TYR	88	10.295	11.941	27.945	1.00	31.78	CPS4
ATOM	3498	C	TYR	88	13.049	17.631	29.105	1.00	20.69	CPS4
ATOM	3499	O	TYR	88	11.839	17.679	28.915	1.00	20.95	CPS4
ATOM	3500	N	ILE	89	13.930	18.130	28.257	1.00	21.21	CPS4
ATOM	3501	CA	ILE	89	13.501	18.805	27.042	1.00	21.24	CPS4
ATOM	3502	CB	ILE	89	14.275	20.141	26.878	1.00	20.12	CPS4
ATOM	3503	CG2	ILE	89	14.157	20.667	25.423	1.00	21.03	CPS4
ATOM	3504	CG1	ILE	89	13.757	21.164	27.900	1.00	20.90	CPS4
ATOM	3505	CD1	ILE	89	14.595	22.440	28.000	1.00	21.80	CPS4
ATOM	3506	C	ILE	89	13.698	18.011	25.767	1.00	22.30	CPS4
ATOM	3507	O	ILE	89	14.685	17.290	25.625	1.00	22.10	CPS4
ATOM	3508	N	ILE	90	12.729	18.126	24.862	1.00	22.64	CPS4
ATOM	3509	CA	ILE	90	12.871	17.544	23.538	1.00	23.23	CPS4
ATOM	3510	CB	ILE	90	11.850	16.413	23.228	1.00	25.32	CPS4
ATOM	3511	CG2	ILE	90	11.987	15.303	24.259	1.00	25.34	CPS4
ATOM	3512	CG1	ILE	90	10.424	16.946	23.187	1.00	27.66	CPS4
ATOM	3513	CD1	ILE	90	9.462	16.003	22.454	1.00	29.92	CPS4
ATOM	3514	C	ILE	90	12.609	18.760	22.654	1.00	23.57	CPS4
ATOM	3515	O	ILE	90	11.780	19.610	22.988	1.00	23.18	CPS4
ATOM	3516	N	CYS	91	13.341	18.892	21.558	1.00	22.32	CPS4
ATOM	3517	CA	CYS	91	13.118	20.042	20.692	1.00	24.32	CPS4
ATOM	3518	CB	CYS	91	14.023	21.209	21.096	1.00	22.65	CPS4
ATOM	3519	SG	CYS	91	15.776	20.862	20.976	1.00	28.76	CPS4
ATOM	3520	C	CYS	91	13.367	19.670	19.244	1.00	24.59	CPS4
ATOM	3521	O	CYS	91	13.834	18.575	18.947	1.00	26.28	CPS4
ATOM	3522	N	THR	92	13.064	20.591	18.344	1.00	25.08	CPS4
ATOM	3523	CA	THR	92	13.234	20.325	16.920	1.00	25.91	CPS4
ATOM	3524	CB	THR	92	12.266	21.187	16.102	1.00	26.21	CPS4
ATOM	3525	OG1	THR	92	12.577	22.562	16.329	1.00	25.10	CPS4
ATOM	3526	CG2	THR	92	10.828	20.933	16.526	1.00	25.78	CPS4
ATOM	3527	C	THR	92	14.633	20.629	16.417	1.00	26.72	CPS4
ATOM	3528	O	THR	92	14.938	20.371	15.255	1.00	27.72	CPS4
ATOM	3529	N	LYS	93	15.480	21.163	17.291	1.00	26.75	CPS4
ATOM	3530	CA	LYS	93	16.830	21.589	16.927	1.00	28.49	CPS4
ATOM	3531	CB	LYS	93	17.109	22.946	17.583	1.00	30.97	CPS4
ATOM	3532	CG	LYS	93	16.792	24.162	16.729	1.00	36.76	CPS4
ATOM	3533	CD	LYS	93	15.450	24.100	16.039	1.00	38.80	CPS4

FIG. 1A-62

ATOM	3534	CE	LYS	93	15.212	25.376	15.229	1.00	40.84	CPS4
ATOM	3535	NZ	LYS	93	14.048	25.250	14.312	1.00	43.58	CPS4
ATOM	3536	C	LYS	93	18.005	20.676	17.234	1.00	27.51	CPS4
ATOM	3537	O	LYS	93	19.005	20.676	16.509	1.00	27.46	CPS4
ATOM	3538	N	LEU	94	17.910	19.911	18.307	1.00	26.01	CPS4
ATOM	3539	CA	LEU	94	19.020	19.058	18.676	1.00	25.30	CPS4
ATOM	3540	CB	LEU	94	20.055	19.904	19.408	1.00	27.33	CPS4
ATOM	3541	CG	LEU	94	19.418	20.843	20.433	1.00	28.62	CPS4
ATOM	3542	CD1	LEU	94	19.228	20.074	21.712	1.00	30.37	CPS4
ATOM	3543	CD2	LEU	94	20.292	22.060	20.673	1.00	30.20	CPS4
ATOM	3544	C	LEU	94	18.556	17.889	19.524	1.00	25.14	CPS4
ATOM	3545	O	LEU	94	17.414	17.854	19.974	1.00	24.61	CPS4
ATOM	3546	N	SER	95	19.460	16.944	19.755	1.00	24.28	CPS4
ATOM	3547	CA	SER	95	19.153	15.731	20.499	1.00	26.04	CPS4
ATOM	3548	CB	SER	95	20.323	14.756	20.355	1.00	27.48	CPS4
ATOM	3549	OG	SER	95	20.100	13.586	21.116	1.00	33.27	CPS4
ATOM	3550	C	SER	95	18.825	15.908	21.982	1.00	25.21	CPS4
ATOM	3551	O	SER	95	19.445	16.714	22.672	1.00	26.64	CPS4
ATOM	3552	N	PRO	96	17.840	15.150	22.485	1.00	25.96	CPS4
ATOM	3553	CD	PRO	96	16.943	14.229	21.760	1.00	25.56	CPS4
ATOM	3554	CA	PRO	96	17.461	15.245	23.900	1.00	26.26	CPS4
ATOM	3555	CB	PRO	96	16.385	14.165	24.045	1.00	26.57	CPS4
ATOM	3556	CG	PRO	96	15.745	14.149	22.679	1.00	27.21	CPS4
ATOM	3557	C	PRO	96	18.677	14.961	24.787	1.00	26.31	CPS4
ATOM	3558	O	PRO	96	18.835	15.561	25.856	1.00	24.59	CPS4
ATOM	3559	N	ALA	97	19.541	14.056	24.323	1.00	27.53	CPS4
ATOM	3560	CA	ALA	97	20.739	13.678	25.074	1.00	29.07	CPS4
ATOM	3561	CB	ALA	97	21.480	12.589	24.286	1.00	34.39	CPS4
ATOM	3562	C	ALA	97	21.690	14.853	25.314	1.00	27.61	CPS4
ATOM	3563	O	ALA	97	22.492	14.827	26.251	1.00	26.14	CPS4
ATOM	3564	N	ALA	98	21.599	15.885	24.483	1.00	24.18	CPS4
ATOM	3565	CA	ALA	98	22.486	17.034	24.617	1.00	23.38	CPS4
ATOM	3566	CB	ALA	98	22.804	17.600	23.238	1.00	25.54	CPS4
ATOM	3567	C	ALA	98	21.943	18.150	25.500	1.00	23.06	CPS4
ATOM	3568	O	ALA	98	22.634	19.140	25.730	1.00	23.28	CPS4
ATOM	3569	N	VAL	99	20.720	17.993	25.999	1.00	21.46	CPS4
ATOM	3570	CA	VAL	99	20.109	19.048	26.796	1.00	20.54	CPS4
ATOM	3571	CB	VAL	99	18.806	19.548	26.146	1.00	21.70	CPS4
ATOM	3572	CG1	VAL	99	18.317	20.837	26.820	1.00	20.11	CPS4
ATOM	3573	CG2	VAL	99	19.026	19.777	24.692	1.00	25.15	CPS4
ATOM	3574	C	VAL	99	19.781	18.622	28.206	1.00	20.45	CPS4
ATOM	3575	O	VAL	99	19.399	17.477	28.450	1.00	20.26	CPS4
ATOM	3576	N	HIS	100	19.924	19.572	29.123	1.00	19.96	CPS4
ATOM	3577	CA	HIS	100	19.634	19.349	30.531	1.00	19.64	CPS4
ATOM	3578	CB	HIS	100	20.935	19.210	31.318	1.00	20.91	CPS4
ATOM	3579	CG	HIS	100	21.844	18.154	30.773	1.00	24.67	CPS4
ATOM	3580	CD2	HIS	100	22.842	18.227	29.862	1.00	26.77	CPS4
ATOM	3581	ND1	HIS	100	21.715	16.820	31.096	1.00	26.53	CPS4
ATOM	3582	CE1	HIS	100	22.593	16.115	30.403	1.00	26.82	CPS4
ATOM	3583	NE2	HIS	100	23.288	16.946	29.646	1.00	28.13	CPS4
ATOM	3584	C	HIS	100	18.864	20.561	31.020	1.00	18.58	CPS4
ATOM	3585	O	HIS	100	19.141	21.683	30.602	1.00	18.37	CPS4
ATOM	3586	N	VAL	101	17.907	20.336	31.911	1.00	18.87	CPS4
ATOM	3587	CA	VAL	101	17.103	21.434	32.431	1.00	17.84	CPS4
ATOM	3588	CB	VAL	101	15.800	21.590	31.608	1.00	16.78	CPS4
ATOM	3589	CG1	VAL	101	14.930	20.345	31.770	1.00	18.44	CPS4
ATOM	3590	CG2	VAL	101	15.029	22.840	32.049	1.00	18.77	CPS4

FIG. 1A-63

ATOM	3591	C	VAL	101	16.723	21.199	33.879	1.00	18.74	CPS4
ATOM	3592	O	VAL	101	16.711	20.069	34.350	1.00	17.29	CPS4
ATOM	3593	N	SER	102	16.441	22.287	34.590	1.00	18.62	CPS4
ATOM	3594	CA	SER	102	15.980	22.193	35.963	1.00	18.53	CPS4
ATOM	3595	CB	SER	102	17.117	22.333	36.970	1.00	19.00	CPS4
ATOM	3596	OG	SER	102	16.596	22.169	38.289	1.00	19.73	CPS4
ATOM	3597	C	SER	102	15.004	23.348	36.139	1.00	19.67	CPS4
ATOM	3598	O	SER	102	15.250	24.446	35.638	1.00	18.04	CPS4
ATOM	3599	N	ILE	103	13.901	23.092	36.841	1.00	19.50	CPS4
ATOM	3600	CA	ILE	103	12.886	24.105	37.082	1.00	19.92	CPS4
ATOM	3601	CB	ILE	103	11.552	23.731	36.386	1.00	22.07	CPS4
ATOM	3602	CG2	ILE	103	10.527	24.867	36.551	1.00	23.01	CPS4
ATOM	3603	CG1	ILE	103	11.804	23.454	34.905	1.00	21.39	CPS4
ATOM	3604	CD1	ILE	103	10.570	22.958	34.144	1.00	21.32	CPS4
ATOM	3605	C	ILE	103	12.642	24.173	38.590	1.00	20.11	CPS4
ATOM	3606	O	ILE	103	12.633	23.137	39.277	1.00	20.14	CPS4
ATOM	3607	N	THR	104	12.462	25.386	39.098	1.00	18.69	CPS4
ATOM	3608	CA	THR	104	12.205	25.588	40.517	1.00	21.54	CPS4
ATOM	3609	CB	THR	104	13.492	26.019	41.274	1.00	23.15	CPS4
ATOM	3610	OG1	THR	104	13.245	26.008	42.686	1.00	23.24	CPS4
ATOM	3611	CG2	THR	104	13.927	27.418	40.856	1.00	22.71	CPS4
ATOM	3612	C	THR	104	11.113	26.639	40.698	1.00	21.91	CPS4
ATOM	3613	O	THR	104	10.790	27.376	39.772	1.00	19.56	CPS4
ATOM	3614	N	HIS	105	10.542	26.701	41.899	1.00	22.60	CPS4
ATOM	3615	CA	HIS	105	9.465	27.639	42.189	1.00	24.01	CPS4
ATOM	3616	CB	HIS	105	8.110	26.927	42.112	1.00	26.53	CPS4
ATOM	3617	CG	HIS	105	7.721	26.457	40.746	1.00	30.77	CPS4
ATOM	3618	CD2	HIS	105	7.892	25.262	40.130	1.00	32.51	CPS4
ATOM	3619	ND1	HIS	105	6.995	27.237	39.871	1.00	32.62	CPS4
ATOM	3620	CE1	HIS	105	6.731	26.543	38.778	1.00	32.63	CPS4
ATOM	3621	NE2	HIS	105	7.264	25.341	38.909	1.00	33.46	CPS4
ATOM	3622	C	HIS	105	9.558	28.179	43.613	1.00	24.17	CPS4
ATOM	3623	O	HIS	105	10.135	27.537	44.491	1.00	22.69	CPS4
ATOM	3624	N	THR	106	8.992	29.366	43.816	1.00	24.57	CPS4
ATOM	3625	CA	THR	106	8.856	29.967	45.147	1.00	24.52	CPS4
ATOM	3626	CB	THR	106	9.756	31.195	45.408	1.00	24.79	CPS4
ATOM	3627	OG1	THR	106	9.327	32.299	44.602	1.00	23.92	CPS4
ATOM	3628	CG2	THR	106	11.210	30.858	45.127	1.00	24.13	CPS4
ATOM	3629	C	THR	106	7.415	30.444	45.065	1.00	26.14	CPS4
ATOM	3630	O	THR	106	6.756	30.249	44.034	1.00	26.11	CPS4
ATOM	3631	N	LYS	107	6.917	31.072	46.123	1.00	26.83	CPS4
ATOM	3632	CA	LYS	107	5.539	31.546	46.115	1.00	27.90	CPS4
ATOM	3633	CB	LYS	107	5.200	32.186	47.464	1.00	30.86	CPS4
ATOM	3634	CG	LYS	107	3.756	32.658	47.573	1.00	34.83	CPS4
ATOM	3635	CD	LYS	107	3.490	33.278	48.940	1.00	39.94	CPS4
ATOM	3636	CE	LYS	107	2.024	33.649	49.117	1.00	42.44	CPS4
ATOM	3637	NZ	LYS	107	1.755	34.215	50.479	1.00	45.42	CPS4
ATOM	3638	C	LYS	107	5.250	32.541	44.994	1.00	26.50	CPS4
ATOM	3639	O	LYS	107	4.169	32.511	44.402	1.00	27.10	CPS4
ATOM	3640	N	GLU	108	6.222	33.396	44.684	1.00	24.12	CPS4
ATOM	3641	CA	GLU	108	6.050	34.436	43.672	1.00	23.55	CPS4
ATOM	3642	CB	GLU	108	6.476	35.783	44.256	1.00	27.75	CPS4
ATOM	3643	CG	GLU	108	5.755	36.152	45.530	1.00	34.21	CPS4
ATOM	3644	CD	GLU	108	4.301	36.440	45.297	1.00	39.02	CPS4
ATOM	3645	OE1	GLU	108	3.639	35.645	44.593	1.00	43.65	CPS4
ATOM	3646	OE2	GLU	108	3.813	37.463	45.823	1.00	44.70	CPS4
ATOM	3647	C	GLU	108	6.794	34.267	42.352	1.00	23.22	CPS4

FIG. 1A-64

ATOM	3648	O	GLU	108	6.553	35.023	41.400	1.00 22.15	CPS4
ATOM	3649	N	TYR	109	7.711	33.308	42.293	1.00 21.80	CPS4
ATOM	3650	CA	TYR	109	8.509	33.129	41.077	1.00 22.23	CPS4
ATOM	3651	CB	TYR	109	9.940	33.626	41.317	1.00 22.18	CPS4
ATOM	3652	CG	TYR	109	10.035	35.082	41.674	1.00 22.99	CPS4
ATOM	3653	CD1	TYR	109	9.984	36.062	40.688	1.00 22.71	CPS4
ATOM	3654	CE1	TYR	109	10.017	37.418	41.018	1.00 25.19	CPS4
ATOM	3655	CD2	TYR	109	10.127	35.485	43.008	1.00 25.01	CPS4
ATOM	3656	CE2	TYR	109	10.158	36.833	43.350	1.00 26.56	CPS4
ATOM	3657	CZ	TYR	109	10.101	37.793	42.349	1.00 26.58	CPS4
ATOM	3658	OH	TYR	109	10.114	39.128	42.677	1.00 29.10	CPS4
ATOM	3659	C	TYR	109	8.625	31.713	40.569	1.00 20.65	CPS4
ATOM	3660	O	TYR	109	8.402	30.757	41.297	1.00 20.79	CPS4
ATOM	3661	N	ALA	110	8.989	31.609	39.294	1.00 21.05	CPS4
ATOM	3662	CA	ALA	110	9.280	30.334	38.654	1.00 19.88	CPS4
ATOM	3663	CB	ALA	110	8.267	29.999	37.567	1.00 21.21	CPS4
ATOM	3664	C	ALA	110	10.638	30.617	38.028	1.00 19.33	CPS4
ATOM	3665	O	ALA	110	10.887	31.730	37.568	1.00 20.58	CPS4
ATOM	3666	N	ALA	111	11.525	29.626	38.008	1.00 18.54	CPS4
ATOM	3667	CA	ALA	111	12.842	29.834	37.423	1.00 17.54	CPS4
ATOM	3668	CB	ALA	111	13.840	30.291	38.498	1.00 17.07	CPS4
ATOM	3669	C	ALA	111	13.314	28.540	36.786	1.00 16.63	CPS4
ATOM	3670	O	ALA	111	12.873	27.454	37.160	1.00 17.51	CPS4
ATOM	3671	N	ALA	112	14.218	28.654	35.826	1.00 17.15	CPS4
ATOM	3672	CA	ALA	112	14.721	27.471	35.161	1.00 16.51	CPS4
ATOM	3673	CB	ALA	112	13.771	27.054	34.046	1.00 17.29	CPS4
ATOM	3674	C	ALA	112	16.092	27.742	34.583	1.00 16.61	CPS4
ATOM	3675	O	ALA	112	16.476	28.887	34.363	1.00 15.97	CPS4
ATOM	3676	N	GLN	113	16.842	26.677	34.356	1.00 17.66	CPS4
ATOM	3677	CA	GLN	113	18.148	26.829	33.754	1.00 17.26	CPS4
ATOM	3678	CB	GLN	113	19.257	26.820	34.811	1.00 19.62	CPS4
ATOM	3679	CG	GLN	113	19.419	25.510	35.538	1.00 23.20	CPS4
ATOM	3680	CD	GLN	113	20.569	25.522	36.537	1.00 26.68	CPS4
ATOM	3681	OE1	GLN	113	20.942	24.480	37.077	1.00 29.56	CPS4
ATOM	3682	NE2	GLN	113	21.121	26.697	36.798	1.00 29.78	CPS4
ATOM	3683	C	GLN	113	18.314	25.678	32.789	1.00 17.26	CPS4
ATOM	3684	O	GLN	113	17.741	24.609	32.975	1.00 16.60	CPS4
ATOM	3685	N	VAL	114	19.093	25.910	31.746	1.00 16.61	CPS4
ATOM	3686	CA	VAL	114	19.329	24.880	30.744	1.00 17.56	CPS4
ATOM	3687	CB	VAL	114	18.523	25.161	29.436	1.00 17.29	CPS4
ATOM	3688	CG1	VAL	114	19.016	24.268	28.275	1.00 18.95	CPS4
ATOM	3689	CG2	VAL	114	17.058	24.895	29.671	1.00 19.12	CPS4
ATOM	3690	C	VAL	114	20.795	24.886	30.386	1.00 17.66	CPS4
ATOM	3691	O	VAL	114	21.454	25.938	30.404	1.00 17.69	CPS4
ATOM	3692	N	VAL	115	21.309	23.696	30.104	1.00 18.00	CPS4
ATOM	3693	CA	VAL	115	22.673	23.566	29.629	1.00 18.27	CPS4
ATOM	3694	CB	VAL	115	23.611	22.872	30.635	1.00 19.25	CPS4
ATOM	3695	CG1	VAL	115	24.962	22.560	29.939	1.00 19.98	CPS4
ATOM	3696	CG2	VAL	115	23.845	23.762	31.841	1.00 17.55	CPS4
ATOM	3697	C	VAL	115	22.597	22.696	28.378	1.00 19.07	CPS4
ATOM	3698	O	VAL	115	21.987	21.626	28.394	1.00 20.13	CPS4
ATOM	3699	N	ILE	116	23.197	23.170	27.293	1.00 18.54	CPS4
ATOM	3700	CA	ILE	116	23.236	22.407	26.053	1.00 21.10	CPS4
ATOM	3701	CB	ILE	116	22.762	23.239	24.850	1.00 21.01	CPS4
ATOM	3702	CG2	ILE	116	22.921	22.420	23.563	1.00 20.56	CPS4
ATOM	3703	CG1	ILE	116	21.298	23.652	25.046	1.00 19.07	CPS4
ATOM	3704	CD1	ILE	116	20.775	24.599	23.943	1.00 18.68	CPS4

FIG. 1A-65

ATOM	3705	C	ILE	116	24.692	22.029	25.851	1.00	22.03	CPS4
ATOM	3706	O	ILE	116	25.570	22.884	25.856	1.00	21.24	CPS4
ATOM	3707	N	GLU	117	24.951	20.736	25.702	1.00	25.15	CPS4
ATOM	3708	CA	GLU	117	26.317	20.266	25.509	1.00	28.51	CPS4
ATOM	3709	CB	GLU	117	26.469	18.835	26.012	1.00	28.70	CPS4
ATOM	3710	CG	GLU	117	26.237	18.661	27.490	1.00	33.10	CPS4
ATOM	3711	CD	GLU	117	26.513	17.240	27.929	1.00	34.43	CPS4
ATOM	3712	OE1	GLU	117	27.702	16.908	28.114	1.00	36.09	CPS4
ATOM	3713	OE2	GLU	117	25.545	16.458	28.070	1.00	35.59	CPS4
ATOM	3714	C	GLU	117	26.677	20.279	24.041	1.00	30.50	CPS4
ATOM	3715	O	GLU	117	25.815	20.420	23.186	1.00	29.91	CPS4
ATOM	3716	N	ARG	118	27.960	20.137	23.747	1.00	34.16	CPS4
ATOM	3717	CA	ARG	118	28.371	20.085	22.355	1.00	38.48	CPS4
ATOM	3718	CB	ARG	118	29.800	20.597	22.182	1.00	41.53	CPS4
ATOM	3719	CG	ARG	118	29.971	22.069	22.549	1.00	45.64	CPS4
ATOM	3720	CD	ARG	118	30.881	22.808	21.567	1.00	47.97	CPS4
ATOM	3721	NE	ARG	118	30.154	23.472	20.477	1.00	50.66	CPS4
ATOM	3722	CZ	ARG	118	29.372	22.860	19.585	1.00	50.73	CPS4
ATOM	3723	NH1	ARG	118	29.188	21.550	19.633	1.00	52.65	CPS4
ATOM	3724	NH2	ARG	118	28.786	23.560	18.622	1.00	51.12	CPS4
ATOM	3725	C	ARG	118	28.285	18.615	21.984	1.00	40.15	CPS4
ATOM	3726	OT1	ARG	118	27.421	18.274	21.156	1.00	41.62	CPS4
ATOM	3727	OT2	ARG	118	29.063	17.816	22.555	1.00	41.20	CPS4
ATOM	3728	C	GLY	1	28.742	14.952	31.117	1.00	33.66	CPS5
ATOM	3729	O	GLY	1	29.119	14.581	32.234	1.00	34.07	CPS5
ATOM	3730	N	GLY	1	30.561	13.536	30.129	1.00	37.12	CPS5
ATOM	3731	CA	GLY	1	29.506	14.565	29.858	1.00	34.50	CPS5
ATOM	3732	N	ILE	2	27.654	15.692	30.948	1.00	31.08	CPS5
ATOM	3733	CA	ILE	2	26.856	16.110	32.095	1.00	28.11	CPS5
ATOM	3734	CB	ILE	2	26.178	17.462	31.826	1.00	27.63	CPS5
ATOM	3735	CG2	ILE	2	25.128	17.747	32.899	1.00	24.45	CPS5
ATOM	3736	CG1	ILE	2	27.244	18.559	31.785	1.00	28.90	CPS5
ATOM	3737	CD1	ILE	2	26.695	19.935	31.484	1.00	31.41	CPS5
ATOM	3738	C	ILE	2	25.797	15.083	32.441	1.00	27.43	CPS5
ATOM	3739	O	ILE	2	25.067	14.611	31.567	1.00	27.84	CPS5
ATOM	3740	N	TYR	3	25.719	14.735	33.723	1.00	27.08	CPS5
ATOM	3741	CA	TYR	3	24.737	13.768	34.198	1.00	27.10	CPS5
ATOM	3742	CB	TYR	3	25.220	13.087	35.476	1.00	30.18	CPS5
ATOM	3743	CG	TYR	3	24.212	12.108	36.033	1.00	34.88	CPS5
ATOM	3744	CD1	TYR	3	24.012	10.862	35.428	1.00	36.41	CPS5
ATOM	3745	CE1	TYR	3	23.063	9.963	35.920	1.00	38.43	CPS5
ATOM	3746	CD2	TYR	3	23.435	12.433	37.146	1.00	36.11	CPS5
ATOM	3747	CE2	TYR	3	22.484	11.542	37.646	1.00	38.38	CPS5
ATOM	3748	CZ	TYR	3	22.305	10.309	37.029	1.00	39.52	CPS5
ATOM	3749	OH	TYR	3	21.378	9.418	37.530	1.00	42.62	CPS5
ATOM	3750	C	TYR	3	23.418	14.475	34.485	1.00	26.49	CPS5
ATOM	3751	O	TYR	3	22.340	13.985	34.130	1.00	24.87	CPS5
ATOM	3752	N	GLY	4	23.499	15.624	35.153	1.00	24.12	CPS5
ATOM	3753	CA	GLY	4	22.284	16.355	35.449	1.00	22.31	CPS5
ATOM	3754	C	GLY	4	22.562	17.715	36.047	1.00	20.04	CPS5
ATOM	3755	O	GLY	4	23.667	17.966	36.509	1.00	20.64	CPS5
ATOM	3756	N	ILE	5	21.572	18.602	36.011	1.00	19.86	CPS5
ATOM	3757	CA	ILE	5	21.730	19.932	36.592	1.00	18.90	CPS5
ATOM	3758	CB	ILE	5	21.865	21.055	35.523	1.00	18.93	CPS5
ATOM	3759	CG2	ILE	5	22.936	20.676	34.510	1.00	18.22	CPS5
ATOM	3760	CG1	ILE	5	20.521	21.321	34.835	1.00	19.13	CPS5
ATOM	3761	CD1	ILE	5	20.582	22.454	33.780	1.00	18.31	CPS5

FIG. 1A-66

ATOM	3762	C	ILE	5	20.532	20.234	37.471	1.00	18.47	CPS5
ATOM	3763	O	ILE	5	19.456	19.655	37.309	1.00	17.95	CPS5
ATOM	3764	N	GLY	6	20.727	21.149	38.410	1.00	18.51	CPS5
ATOM	3765	CA	GLY	6	19.654	21.489	39.318	1.00	18.44	CPS5
ATOM	3766	C	GLY	6	19.741	22.925	39.766	1.00	18.43	CPS5
ATOM	3767	O	GLY	6	20.829	23.461	39.972	1.00	18.58	CPS5
ATOM	3768	N	LEU	7	18.572	23.530	39.916	1.00	17.51	CPS5
ATOM	3769	CA	LEU	7	18.429	24.910	40.337	1.00	18.75	CPS5
ATOM	3770	CB	LEU	7	17.977	25.769	39.146	1.00	20.12	CPS5
ATOM	3771	CG	LEU	7	17.715	27.246	39.457	1.00	20.05	CPS5
ATOM	3772	CD1	LEU	7	19.056	27.945	39.706	1.00	18.90	CPS5
ATOM	3773	CD2	LEU	7	16.967	27.907	38.298	1.00	19.78	CPS5
ATOM	3774	C	LEU	7	17.366	24.991	41.428	1.00	19.75	CPS5
ATOM	3775	O	LEU	7	16.329	24.330	41.353	1.00	18.94	CPS5
ATOM	3776	N	ASP	8	17.626	25.797	42.450	1.00	18.42	CPS5
ATOM	3777	CA	ASP	8	16.644	25.985	43.491	1.00	20.59	CPS5
ATOM	3778	CB	ASP	8	16.823	24.969	44.625	1.00	22.60	CPS5
ATOM	3779	CG	ASP	8	15.838	25.199	45.764	1.00	25.07	CPS5
ATOM	3780	OD1	ASP	8	16.142	26.008	46.666	1.00	26.32	CPS5
ATOM	3781	OD2	ASP	8	14.749	24.597	45.742	1.00	26.96	CPS5
ATOM	3782	C	ASP	8	16.700	27.391	44.066	1.00	19.95	CPS5
ATOM	3783	O	ASP	8	17.768	27.957	44.243	1.00	21.00	CPS5
ATOM	3784	N	ILE	9	15.533	27.966	44.309	1.00	19.58	CPS5
ATOM	3785	CA	ILE	9	15.456	29.275	44.949	1.00	19.88	CPS5
ATOM	3786	CB	ILE	9	14.814	30.352	44.055	1.00	19.43	CPS5
ATOM	3787	CG2	ILE	9	14.757	31.674	44.820	1.00	19.92	CPS5
ATOM	3788	CG1	ILE	9	15.640	30.524	42.776	1.00	18.89	CPS5
ATOM	3789	CD1	ILE	9	15.018	31.488	41.770	1.00	19.11	CPS5
ATOM	3790	C	ILE	9	14.538	29.012	46.121	1.00	20.96	CPS5
ATOM	3791	O	ILE	9	13.482	28.392	45.964	1.00	20.32	CPS5
ATOM	3792	N	THR	10	14.950	29.453	47.301	1.00	20.95	CPS5
ATOM	3793	CA	THR	10	14.145	29.250	48.491	1.00	22.53	CPS5
ATOM	3794	CB	THR	10	14.837	28.265	49.452	1.00	23.91	CPS5
ATOM	3795	OG1	THR	10	14.913	26.976	48.821	1.00	24.32	CPS5
ATOM	3796	CG2	THR	10	14.045	28.138	50.764	1.00	24.45	CPS5
ATOM	3797	C	THR	10	13.893	30.567	49.207	1.00	23.06	CPS5
ATOM	3798	O	THR	10	14.810	31.375	49.398	1.00	22.57	CPS5
ATOM	3799	N	GLU	11	12.641	30.782	49.588	1.00	23.52	CPS5
ATOM	3800	CA	GLU	11	12.260	31.997	50.302	1.00	24.89	CPS5
ATOM	3801	CB	GLU	11	10.747	32.212	50.168	1.00	25.23	CPS5
ATOM	3802	CG	GLU	11	10.217	33.456	50.870	1.00	27.69	CPS5
ATOM	3803	CD	GLU	11	8.701	33.491	50.901	1.00	29.32	CPS5
ATOM	3804	OE1	GLU	11	8.079	32.418	50.756	1.00	30.90	CPS5
ATOM	3805	OE2	GLU	11	8.129	34.584	51.089	1.00	33.76	CPS5
ATOM	3806	C	GLU	11	12.668	31.858	51.781	1.00	24.72	CPS5
ATOM	3807	O	GLU	11	12.246	30.925	52.469	1.00	25.10	CPS5
ATOM	3808	N	LEU	12	13.510	32.772	52.252	1.00	24.85	CPS5
ATOM	3809	CA	LEU	12	13.988	32.756	53.633	1.00	24.83	CPS5
ATOM	3810	CB	LEU	12	14.850	33.997	53.895	1.00	25.59	CPS5
ATOM	3811	CG	LEU	12	16.371	33.834	53.933	1.00	28.80	CPS5
ATOM	3812	CD1	LEU	12	16.851	32.954	52.799	1.00	28.80	CPS5
ATOM	3813	CD2	LEU	12	17.018	35.199	53.858	1.00	30.41	CPS5
ATOM	3814	C	LEU	12	12.856	32.691	54.661	1.00	26.18	CPS5
ATOM	3815	O	LEU	12	12.947	31.983	55.658	1.00	25.34	CPS5
ATOM	3816	N	LYS	13	11.788	33.432	54.403	1.00	27.19	CPS5
ATOM	3817	CA	LYS	13	10.644	33.479	55.304	1.00	29.15	CPS5
ATOM	3818	CB	LYS	13	9.634	34.508	54.777	1.00	31.29	CPS5

FIG. 1A-67


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ATOM   3819  CG  LYS  13       8.429  34.734  55.668  1.00 36.36      CPS5
ATOM   3820  CD  LYS  13       7.596  35.907  55.154  1.00 40.04      CPS5
ATOM   3821  CE  LYS  13       6.387  36.178  56.041  1.00 42.34      CPS5
ATOM   3822  NZ  LYS  13       5.660  37.416  55.611  1.00 44.27      CPS5
ATOM   3823  C   LYS  13       9.989  32.108  55.449  1.00 29.23      CPS5
ATOM   3824  O   LYS  13       9.513  31.742  56.525  1.00 27.84      CPS5
ATOM   3825  N   ARG  14       9.971  31.345  54.362  1.00 28.90      CPS5
ATOM   3826  CA  ARG  14       9.371  30.019  54.384  1.00 29.32      CPS5
ATOM   3827  CB  ARG  14       9.264  29.486  52.958  1.00 30.67      CPS5
ATOM   3828  CG  ARG  14       8.489  28.186  52.828  1.00 33.67      CPS5
ATOM   3829  CD  ARG  14       8.693  27.591  51.442  1.00 36.77      CPS5
ATOM   3830  NE  ARG  14       8.435  26.157  51.442  1.00 40.83      CPS5
ATOM   3831  CZ  ARG  14       9.204  25.259  50.836  1.00 42.06      CPS5
ATOM   3832  NH1 ARG  14      10.289  25.640  50.176  1.00 40.50      CPS5
ATOM   3833  NH2 ARG  14       8.882  23.973  50.891  1.00 43.70      CPS5
ATOM   3834  C   ARG  14      10.210  29.072  55.257  1.00 28.72      CPS5
ATOM   3835  O   ARG  14       9.665  28.242  55.994  1.00 28.02      CPS5
ATOM   3836  N   ILE  15      11.533  29.199  55.170  1.00 28.10      CPS5
ATOM   3837  CA  ILE  15      12.439  28.378  55.972  1.00 27.56      CPS5
ATOM   3838  CB  ILE  15      13.916  28.640  55.587  1.00 28.43      CPS5
ATOM   3839  CG2 ILE  15      14.863  28.021  56.623  1.00 27.74      CPS5
ATOM   3840  CG1 ILE  15      14.201  28.042  54.204  1.00 26.73      CPS5
ATOM   3841  CD1 ILE  15      14.052  26.517  54.159  1.00 29.51      CPS5
ATOM   3842  C   ILE  15      12.226  28.739  57.441  1.00 29.85      CPS5
ATOM   3843  O   ILE  15      12.131  27.860  58.300  1.00 28.01      CPS5
ATOM   3844  N   ALA  16      12.145  30.039  57.724  1.00 30.25      CPS5
ATOM   3845  CA  ALA  16      11.929  30.508  59.097  1.00 31.84      CPS5
ATOM   3846  CB  ALA  16      11.937  32.038  59.142  1.00 31.96      CPS5
ATOM   3847  C   ALA  16      10.607  29.966  59.644  1.00 32.73      CPS5
ATOM   3848  O   ALA  16      10.534  29.550  60.802  1.00 33.57      CPS5
ATOM   3849  N   SER  17       9.564  29.958  58.820  1.00 33.10      CPS5
ATOM   3850  CA  SER  17       8.276  29.435  59.269  1.00 35.41      CPS5
ATOM   3851  CB  SER  17       7.206  29.639  58.201  1.00 36.49      CPS5
ATOM   3852  OG  SER  17       6.988  31.024  57.990  1.00 40.91      CPS5
ATOM   3853  C   SER  17       8.369  27.954  59.617  1.00 35.50      CPS5
ATOM   3854  O   SER  17       7.938  27.532  60.696  1.00 35.16      CPS5
ATOM   3855  N   MET  18       8.927  27.164  58.705  1.00 35.27      CPS5
ATOM   3856  CA  MET  18       9.073  25.731  58.942  1.00 36.03      CPS5
ATOM   3857  CB  MET  18       9.701  25.045  57.726  1.00 36.24      CPS5
ATOM   3858  CG  MET  18       8.794  24.994  56.519  1.00 38.74      CPS5
ATOM   3859  SD  MET  18       9.503  24.027  55.178  1.00 44.39      CPS5
ATOM   3860  CE  MET  18      10.534  25.241  54.428  1.00 38.98      CPS5
ATOM   3861  C   MET  18       9.918  25.462  60.180  1.00 35.92      CPS5
ATOM   3862  O   MET  18       9.597  24.580  60.979  1.00 37.63      CPS5
ATOM   3863  N   ALA  19      10.995  26.220  60.348  1.00 35.18      CPS5
ATOM   3864  CA  ALA  19      11.859  26.033  61.504  1.00 35.87      CPS5
ATOM   3865  CB  ALA  19      13.081  26.932  61.401  1.00 35.73      CPS5
ATOM   3866  C   ALA  19      11.087  26.348  62.783  1.00 38.24      CPS5
ATOM   3867  O   ALA  19      11.367  25.787  63.844  1.00 36.83      CPS5
ATOM   3868  N   GLY  20      10.106  27.239  62.669  1.00 38.64      CPS5
ATOM   3869  CA  GLY  20       9.320  27.619  63.827  1.00 40.77      CPS5
ATOM   3870  C   GLY  20       8.203  26.663  64.196  1.00 41.91      CPS5
ATOM   3871  O   GLY  20       7.826  26.580  65.361  1.00 43.62      CPS5
ATOM   3872  N   ARG  21       7.668  25.935  63.225  1.00 42.69      CPS5
ATOM   3873  CA  ARG  21       6.580  25.012  63.511  1.00 44.15      CPS5
ATOM   3874  CB  ARG  21       5.574  25.026  62.362  1.00 46.42      CPS5
ATOM   3875  CG  ARG  21       6.018  24.224  61.156  1.00 50.19      CPS5
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FIG. 1A-68


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ATOM   3876  CD  ARG  21       5.388  24.747  59.879  1.00 53.16      CPS5
ATOM   3877  NE  ARG  21       5.589  23.833  58.759  1.00 54.93      CPS5
ATOM   3878  CZ  ARG  21       5.372  24.159  57.490  1.00 56.47      CPS5
ATOM   3879  NH1 ARG  21       4.956  25.383  57.184  1.00 57.16      CPS5
ATOM   3880  NH2 ARG  21       5.554  23.258  56.533  1.00 56.82      CPS5
ATOM   3881  C   ARG  21       7.051  23.579  63.753  1.00 44.27      CPS5
ATOM   3882  O   ARG  21       6.367  22.803  64.420  1.00 44.45      CPS5
ATOM   3883  N   GLN  22       8.213  23.226  63.209  1.00 42.85      CPS5
ATOM   3884  CA  GLN  22       8.741  21.874  63.369  1.00 41.63      CPS5
ATOM   3885  CB  GLN  22       9.212  21.351  62.011  1.00 41.96      CPS5
ATOM   3886  CG  GLN  22       8.182  21.567  60.906  1.00 42.25      CPS5
ATOM   3887  CD  GLN  22       8.610  21.008  59.560  1.00 44.24      CPS5
ATOM   3888  OE1 GLN  22       7.988  21.293  58.533  1.00 45.66      CPS5
ATOM   3889  NE2 GLN  22       9.664  20.202  59.557  1.00 42.69      CPS5
ATOM   3890  C   GLN  22       9.882  21.862  64.387  1.00 41.06      CPS5
ATOM   3891  O   GLN  22      10.853  22.607  64.255  1.00 41.24      CPS5
ATOM   3892  N   LYS  23       9.764  20.995  65.390  1.00 39.60      CPS5
ATOM   3893  CA  LYS  23      10.750  20.903  66.466  1.00 38.55      CPS5
ATOM   3894  CB  LYS  23      10.439  19.695  67.357  1.00 39.83      CPS5
ATOM   3895  CG  LYS  23      11.370  19.589  68.551  1.00 41.79      CPS5
ATOM   3896  CD  LYS  23      10.771  18.745  69.654  1.00 43.79      CPS5
ATOM   3897  CE  LYS  23      10.448  17.353  69.161  1.00 44.48      CPS5
ATOM   3898  NZ  LYS  23      10.028  16.518  70.294  1.00 46.17      CPS5
ATOM   3899  C   LYS  23      12.236  20.885  66.106  1.00 37.06      CPS5
ATOM   3900  O   LYS  23      12.982  21.787  66.501  1.00 40.33      CPS5
ATOM   3901  N   ARG  24      12.679  19.862  65.389  1.00 32.83      CPS5
ATOM   3902  CA  ARG  24      14.093  19.767  65.025  1.00 28.69      CPS5
ATOM   3903  CB  ARG  24      14.693  18.448  65.537  1.00 27.47      CPS5
ATOM   3904  CG  ARG  24      15.128  18.477  67.012  1.00 26.46      CPS5
ATOM   3905  CD  ARG  24      15.742  17.141  67.435  1.00 26.25      CPS5
ATOM   3906  NE  ARG  24      14.723  16.093  67.528  1.00 26.94      CPS5
ATOM   3907  CZ  ARG  24      14.061  15.783  68.640  1.00 26.62      CPS5
ATOM   3908  NH1 ARG  24      14.304  16.423  69.781  1.00 28.42      CPS5
ATOM   3909  NH2 ARG  24      13.128  14.851  68.605  1.00 27.58      CPS5
ATOM   3910  C   ARG  24      14.269  19.874  63.519  1.00 26.86      CPS5
ATOM   3911  O   ARG  24      14.863  19.008  62.872  1.00 24.69      CPS5
ATOM   3912  N   PHE  25      13.747  20.953  62.957  1.00 24.39      CPS5
ATOM   3913  CA  PHE  25      13.848  21.148  61.515  1.00 24.06      CPS5
ATOM   3914  CB  PHE  25      13.089  22.408  61.103  1.00 25.10      CPS5
ATOM   3915  CG  PHE  25      13.220  22.738  59.645  1.00 25.01      CPS5
ATOM   3916  CD1 PHE  25      14.065  23.754  59.224  1.00 26.44      CPS5
ATOM   3917  CD2 PHE  25      12.502  22.029  58.695  1.00 26.17      CPS5
ATOM   3918  CE1 PHE  25      14.192  24.063  57.867  1.00 26.84      CPS5
ATOM   3919  CE2 PHE  25      12.624  22.330  57.338  1.00 27.83      CPS5
ATOM   3920  CZ  PHE  25      13.470  23.348  56.929  1.00 26.25      CPS5
ATOM   3921  C   PHE  25      15.289  21.241  61.034  1.00 23.02      CPS5
ATOM   3922  O   PHE  25      15.669  20.583  60.067  1.00 23.63      CPS5
ATOM   3923  N   ALA  26      16.096  22.055  61.702  1.00 21.62      CPS5
ATOM   3924  CA  ALA  26      17.481  22.211  61.272  1.00 22.64      CPS5
ATOM   3925  CB  ALA  26      18.200  23.213  62.171  1.00 21.17      CPS5
ATOM   3926  C   ALA  26      18.203  20.868  61.295  1.00 22.18      CPS5
ATOM   3927  O   ALA  26      18.962  20.542  60.382  1.00 21.14      CPS5
ATOM   3928  N   GLU  27      17.967  20.098  62.356  1.00 21.95      CPS5
ATOM   3929  CA  GLU  27      18.595  18.784  62.499  1.00 22.37      CPS5
ATOM   3930  CB  GLU  27      18.231  18.176  63.862  1.00 21.57      CPS5
ATOM   3931  CG  GLU  27      18.935  18.817  65.089  1.00 23.00      CPS5
ATOM   3932  CD  GLU  27      18.465  20.233  65.452  1.00 24.81      CPS5
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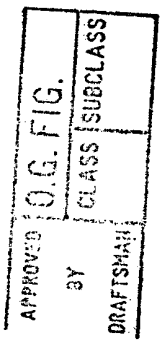
FIG. 1A-69



ATOM	3933	OE1	GLU	27	17.353	20.647	65.056	1.00	23.58	CPS5
ATOM	3934	OE2	GLU	27	19.218	20.932	66.172	1.00	25.05	CPS5
ATOM	3935	C	GLU	27	18.184	17.831	61.369	1.00	23.57	CPS5
ATOM	3936	O	GLU	27	18.937	16.934	61.000	1.00	23.93	CPS5
ATOM	3937	N	ARG	28	16.981	18.015	60.833	1.00	23.21	CPS5
ATOM	3938	CA	ARG	28	16.502	17.173	59.742	1.00	25.30	CPS5
ATOM	3939	CB	ARG	28	14.995	17.391	59.530	1.00	28.97	CPS5
ATOM	3940	CG	ARG	28	14.413	16.636	58.327	1.00	31.14	CPS5
ATOM	3941	CD	ARG	28	12.911	16.353	58.503	1.00	35.90	CPS5
ATOM	3942	NE	ARG	28	12.063	17.535	58.340	1.00	36.29	CPS5
ATOM	3943	CZ	ARG	28	11.774	18.089	57.165	1.00	38.49	CPS5
ATOM	3944	NH1	ARG	28	12.264	17.571	56.045	1.00	37.03	CPS5
ATOM	3945	NH2	ARG	28	10.980	19.154	57.105	1.00	38.67	CPS5
ATOM	3946	C	ARG	28	17.245	17.488	58.439	1.00	24.41	CPS5
ATOM	3947	O	ARG	28	17.582	16.596	57.666	1.00	24.06	CPS5
ATOM	3948	N	ILE	29	17.517	18.765	58.218	1.00	23.36	CPS5
ATOM	3949	CA	ILE	29	18.183	19.212	56.997	1.00	24.49	CPS5
ATOM	3950	CB	ILE	29	17.817	20.693	56.704	1.00	24.90	CPS5
ATOM	3951	CG2	ILE	29	18.374	21.123	55.334	1.00	26.73	CPS5
ATOM	3952	CG1	ILE	29	16.305	20.880	56.773	1.00	24.80	CPS5
ATOM	3953	CD1	ILE	29	15.527	19.982	55.843	1.00	23.16	CPS5
ATOM	3954	C	ILE	29	19.708	19.121	56.983	1.00	24.05	CPS5
ATOM	3955	O	ILE	29	20.313	18.817	55.949	1.00	23.72	CPS5
ATOM	3956	N	LEU	30	20.323	19.383	58.132	1.00	23.56	CPS5
ATOM	3957	CA	LEU	30	21.778	19.444	58.240	1.00	23.33	CPS5
ATOM	3958	CB	LEU	30	22.151	20.701	59.035	1.00	22.47	CPS5
ATOM	3959	CG	LEU	30	21.503	22.020	58.591	1.00	23.18	CPS5
ATOM	3960	CD1	LEU	30	21.940	23.141	59.519	1.00	23.77	CPS5
ATOM	3961	CD2	LEU	30	21.901	22.348	57.157	1.00	22.19	CPS5
ATOM	3962	C	LEU	30	22.492	18.238	58.854	1.00	24.18	CPS5
ATOM	3963	O	LEU	30	21.966	17.577	59.753	1.00	24.62	CPS5
ATOM	3964	N	THR	31	23.704	17.976	58.363	1.00	24.03	CPS5
ATOM	3965	CA	THR	31	24.531	16.878	58.862	1.00	24.72	CPS5
ATOM	3966	CB	THR	31	25.626	16.494	57.850	1.00	25.78	CPS5
ATOM	3967	OG1	THR	31	26.575	17.563	57.761	1.00	26.99	CPS5
ATOM	3968	CG2	THR	31	25.022	16.234	56.466	1.00	24.96	CPS5
ATOM	3969	C	THR	31	25.228	17.351	60.140	1.00	24.37	CPS5
ATOM	3970	O	THR	31	25.134	18.520	60.514	1.00	24.09	CPS5
ATOM	3971	N	ARG	32	25.943	16.452	60.806	1.00	25.54	CPS5
ATOM	3972	CA	ARG	32	26.642	16.832	62.031	1.00	27.17	CPS5
ATOM	3973	CB	ARG	32	27.429	15.651	62.590	1.00	28.99	CPS5
ATOM	3974	CG	ARG	32	26.583	14.597	63.261	1.00	31.34	CPS5
ATOM	3975	CD	ARG	32	27.476	13.684	64.109	1.00	34.50	CPS5
ATOM	3976	NE	ARG	32	26.701	12.698	64.853	1.00	38.58	CPS5
ATOM	3977	CZ	ARG	32	27.200	11.916	65.809	1.00	40.34	CPS5
ATOM	3978	NH1	ARG	32	26.419	11.044	66.435	1.00	37.96	CPS5
ATOM	3979	NH2	ARG	32	28.480	12.009	66.145	1.00	42.21	CPS5
ATOM	3980	C	ARG	32	27.589	18.014	61.865	1.00	27.70	CPS5
ATOM	3981	O	ARG	32	27.562	18.940	62.666	1.00	28.37	CPS5
ATOM	3982	N	SER	33	28.439	17.987	60.841	1.00	27.97	CPS5
ATOM	3983	CA	SER	33	29.379	19.088	60.652	1.00	28.23	CPS5
ATOM	3984	CB	SER	33	30.397	18.746	59.556	1.00	30.14	CPS5
ATOM	3985	OG	SER	33	29.759	18.525	58.309	1.00	34.75	CPS5
ATOM	3986	C	SER	33	28.661	20.398	60.330	1.00	27.70	CPS5
ATOM	3987	O	SER	33	29.082	21.464	60.776	1.00	27.19	CPS5
ATOM	3988	N	GLU	34	27.578	20.319	59.560	1.00	27.25	CPS5
ATOM	3989	CA	GLU	34	26.804	21.511	59.212	1.00	27.47	CPS5

FIG. 1A-70

ATOM	3990	CB	GLU	34	25.759	21.171	58.148	1.00	27.07	CPS5
ATOM	3991	CG	GLU	34	26.368	20.872	56.783	1.00	28.76	CPS5
ATOM	3992	CD	GLU	34	25.376	20.290	55.782	1.00	28.74	CPS5
ATOM	3993	OE1	GLU	34	25.664	20.350	54.569	1.00	31.36	CPS5
ATOM	3994	OE2	GLU	34	24.320	19.764	56.192	1.00	26.92	CPS5
ATOM	3995	C	GLU	34	26.121	22.080	60.454	1.00	27.58	CPS5
ATOM	3996	O	GLU	34	26.028	23.300	60.624	1.00	26.80	CPS5
ATOM	3997	N	LEU	35	25.629	21.196	61.319	1.00	26.86	CPS5
ATOM	3998	CA	LEU	35	24.988	21.653	62.545	1.00	27.86	CPS5
ATOM	3999	CB	LEU	35	24.322	20.476	63.272	1.00	26.37	CPS5
ATOM	4000	CG	LEU	35	23.004	19.992	62.650	1.00	26.60	CPS5
ATOM	4001	CD1	LEU	35	22.597	18.649	63.255	1.00	27.30	CPS5
ATOM	4002	CD2	LEU	35	21.906	21.050	62.890	1.00	25.07	CPS5
ATOM	4003	C	LEU	35	26.032	22.333	63.442	1.00	28.95	CPS5
ATOM	4004	O	LEU	35	25.727	23.317	64.104	1.00	29.27	CPS5
ATOM	4005	N	ASP	36	27.264	21.825	63.458	1.00	31.26	CPS5
ATOM	4006	CA	ASP	36	28.306	22.453	64.279	1.00	33.66	CPS5
ATOM	4007	CB	ASP	36	29.649	21.740	64.127	1.00	36.86	CPS5
ATOM	4008	CG	ASP	36	29.668	20.386	64.795	1.00	39.66	CPS5
ATOM	4009	OD1	ASP	36	28.990	20.235	65.833	1.00	43.45	CPS5
ATOM	4010	OD2	ASP	36	30.373	19.479	64.297	1.00	41.30	CPS5
ATOM	4011	C	ASP	36	28.481	23.905	63.871	1.00	34.39	CPS5
ATOM	4012	O	ASP	36	28.608	24.794	64.722	1.00	34.60	CPS5
ATOM	4013	N	GLN	37	28.488	24.140	62.563	1.00	33.83	CPS5
ATOM	4014	CA	GLN	37	28.639	25.483	62.015	1.00	35.12	CPS5
ATOM	4015	CB	GLN	37	28.809	25.394	60.499	1.00	36.30	CPS5
ATOM	4016	CG	GLN	37	30.079	24.660	60.055	1.00	41.36	CPS5
ATOM	4017	CD	GLN	37	29.944	24.026	58.676	1.00	43.00	CPS5
ATOM	4018	OE1	GLN	37	29.434	24.646	57.746	1.00	44.80	CPS5
ATOM	4019	NE2	GLN	37	30.408	22.786	58.541	1.00	44.26	CPS5
ATOM	4020	C	GLN	37	27.409	26.328	62.344	1.00	34.18	CPS5
ATOM	4021	O	GLN	37	27.513	27.470	62.794	1.00	33.82	CPS5
ATOM	4022	N	TYR	38	26.240	25.736	62.126	1.00	32.84	CPS5
ATOM	4023	CA	TYR	38	24.963	26.395	62.349	1.00	32.66	CPS5
ATOM	4024	CB	TYR	38	23.846	25.419	61.961	1.00	29.71	CPS5
ATOM	4025	CG	TYR	38	22.433	25.884	62.224	1.00	29.29	CPS5
ATOM	4026	CD1	TYR	38	21.721	25.404	63.317	1.00	29.80	CPS5
ATOM	4027	CE1	TYR	38	20.401	25.776	63.541	1.00	31.00	CPS5
ATOM	4028	CD2	TYR	38	21.788	26.763	61.355	1.00	28.96	CPS5
ATOM	4029	CE2	TYR	38	20.459	27.146	61.571	1.00	28.65	CPS5
ATOM	4030	CZ	TYR	38	19.776	26.644	62.665	1.00	29.30	CPS5
ATOM	4031	OH	TYR	38	18.462	26.985	62.885	1.00	28.92	CPS5
ATOM	4032	C	TYR	38	24.746	26.939	63.765	1.00	34.02	CPS5
ATOM	4033	O	TYR	38	24.292	28.068	63.936	1.00	34.37	CPS5
ATOM	4034	N	TYR	39	25.076	26.154	64.780	1.00	36.23	CPS5
ATOM	4035	CA	TYR	39	24.860	26.613	66.144	1.00	38.88	CPS5
ATOM	4036	CB	TYR	39	24.762	25.414	67.082	1.00	38.30	CPS5
ATOM	4037	CG	TYR	39	23.371	24.847	67.036	1.00	38.06	CPS5
ATOM	4038	CD1	TYR	39	22.273	25.658	67.338	1.00	38.93	CPS5
ATOM	4039	CE1	TYR	39	20.974	25.194	67.203	1.00	39.58	CPS5
ATOM	4040	CD2	TYR	39	23.134	23.546	66.608	1.00	37.49	CPS5
ATOM	4041	CE2	TYR	39	21.837	23.064	66.469	1.00	37.88	CPS5
ATOM	4042	CZ	TYR	39	20.760	23.893	66.763	1.00	39.42	CPS5
ATOM	4043	OH	TYR	39	19.470	23.450	66.592	1.00	38.55	CPS5
ATOM	4044	C	TYR	39	25.816	27.658	66.692	1.00	41.19	CPS5
ATOM	4045	O	TYR	39	25.662	28.109	67.822	1.00	42.90	CPS5
ATOM	4046	N	GLU	40	26.789	28.060	65.887	1.00	43.80	CPS5

FIG. 1A-71

ATOM	4047	CA	GLU	40	27.731	29.090	66.304	1.00	46.08	CPS5
ATOM	4048	CB	GLU	40	29.140	28.737	65.834	1.00	48.41	CPS5
ATOM	4049	CG	GLU	40	29.806	27.639	66.639	1.00	52.50	CPS5
ATOM	4050	CD	GLU	40	31.155	27.248	66.063	1.00	54.95	CPS5
ATOM	4051	OE1	GLU	40	31.969	28.154	65.774	1.00	56.23	CPS5
ATOM	4052	OE2	GLU	40	31.403	26.033	65.904	1.00	57.17	CPS5
ATOM	4053	C	GLU	40	27.322	30.446	65.721	1.00	46.24	CPS5
ATOM	4054	O	GLU	40	27.932	31.475	66.023	1.00	46.47	CPS5
ATOM	4055	N	LEU	41	26.279	30.443	64.896	1.00	45.08	CPS5
ATOM	4056	CA	LEU	41	25.803	31.664	64.254	1.00	44.90	CPS5
ATOM	4057	CB	LEU	41	25.304	31.348	62.840	1.00	44.02	CPS5
ATOM	4058	CG	LEU	41	26.227	30.623	61.859	1.00	43.61	CPS5
ATOM	4059	CD1	LEU	41	25.443	30.306	60.591	1.00	42.67	CPS5
ATOM	4060	CD2	LEU	41	27.439	31.480	61.530	1.00	43.84	CPS5
ATOM	4061	C	LEU	41	24.685	32.376	65.013	1.00	45.61	CPS5
ATOM	4062	O	LEU	41	24.021	31.789	65.869	1.00	45.79	CPS5
ATOM	4063	N	SER	42	24.479	33.648	64.677	1.00	46.42	CPS5
ATOM	4064	CA	SER	42	23.432	34.456	65.288	1.00	47.43	CPS5
ATOM	4065	CB	SER	42	23.615	35.924	64.915	1.00	48.22	CPS5
ATOM	4066	OG	SER	42	23.440	36.106	63.520	1.00	48.72	CPS5
ATOM	4067	C	SER	42	22.105	33.963	64.734	1.00	47.92	CPS5
ATOM	4068	O	SER	42	22.081	33.205	63.763	1.00	47.71	CPS5
ATOM	4069	N	GLU	43	21.000	34.399	65.328	1.00	48.18	CPS5
ATOM	4070	CA	GLU	43	19.689	33.959	64.861	1.00	48.69	CPS5
ATOM	4071	CB	GLU	43	18.581	34.563	65.728	1.00	50.88	CPS5
ATOM	4072	CG	GLU	43	17.286	33.765	65.683	1.00	53.85	CPS5
ATOM	4073	CD	GLU	43	16.099	34.579	65.201	1.00	56.30	CPS5
ATOM	4074	OE1	GLU	43	16.189	35.176	64.105	1.00	57.99	CPS5
ATOM	4075	OE2	GLU	43	15.073	34.614	65.916	1.00	56.86	CPS5
ATOM	4076	C	GLU	43	19.449	34.308	63.389	1.00	47.59	CPS5
ATOM	4077	O	GLU	43	18.899	33.503	62.635	1.00	46.68	CPS5
ATOM	4078	N	LYS	44	19.861	35.504	62.979	1.00	46.55	CPS5
ATOM	4079	CA	LYS	44	19.680	35.926	61.591	1.00	46.07	CPS5
ATOM	4080	CB	LYS	44	19.973	37.422	61.439	1.00	47.29	CPS5
ATOM	4081	CG	LYS	44	19.730	37.935	60.031	1.00	49.35	CPS5
ATOM	4082	CD	LYS	44	20.148	39.384	59.857	1.00	50.89	CPS5
ATOM	4083	CE	LYS	44	19.837	39.855	58.440	1.00	52.29	CPS5
ATOM	4084	NZ	LYS	44	20.265	41.261	58.188	1.00	53.26	CPS5
ATOM	4085	C	LYS	44	20.597	35.130	60.660	1.00	44.52	CPS5
ATOM	4086	O	LYS	44	20.185	34.698	59.579	1.00	43.62	CPS5
ATOM	4087	N	ARG	45	21.842	34.944	61.084	1.00	42.61	CPS5
ATOM	4088	CA	ARG	45	22.816	34.195	60.297	1.00	41.42	CPS5
ATOM	4089	CB	ARG	45	24.193	34.284	60.957	1.00	43.69	CPS5
ATOM	4090	CG	ARG	45	25.001	35.512	60.552	1.00	47.18	CPS5
ATOM	4091	CD	ARG	45	26.039	35.120	59.517	1.00	50.46	CPS5
ATOM	4092	NE	ARG	45	25.455	34.243	58.506	1.00	53.21	CPS5
ATOM	4093	CZ	ARG	45	26.141	33.355	57.794	1.00	54.22	CPS5
ATOM	4094	NH1	ARG	45	27.450	33.219	57.975	1.00	54.73	CPS5
ATOM	4095	NH2	ARG	45	25.514	32.593	56.909	1.00	54.37	CPS5
ATOM	4096	C	ARG	45	22.385	32.735	60.156	1.00	39.25	CPS5
ATOM	4097	O	ARG	45	22.620	32.100	59.128	1.00	37.24	CPS5
ATOM	4098	N	LYS	46	21.748	32.209	61.196	1.00	36.43	CPS5
ATOM	4099	CA	LYS	46	21.273	30.830	61.175	1.00	34.18	CPS5
ATOM	4100	CB	LYS	46	20.618	30.472	62.511	1.00	34.58	CPS5
ATOM	4101	CG	LYS	46	21.608	30.164	63.630	1.00	35.23	CPS5
ATOM	4102	CD	LYS	46	20.871	29.751	64.894	1.00	37.58	CPS5
ATOM	4103	CE	LYS	46	21.842	29.392	66.010	1.00	39.36	CPS5

FIG. 1A-72

ATOM	4104	NZ	LYS	46	21.100	29.022	67.241	1.00	40.50	CPS5
ATOM	4105	C	LYS	46	20.267	30.612	60.047	1.00	33.30	CPS5
ATOM	4106	O	LYS	46	20.350	29.631	59.310	1.00	31.70	CPS5
ATOM	4107	N	ASN	47	19.313	31.531	59.924	1.00	31.25	CPS5
ATOM	4108	CA	ASN	47	18.295	31.424	58.892	1.00	30.79	CPS5
ATOM	4109	CB	ASN	47	17.298	32.575	59.020	1.00	32.61	CPS5
ATOM	4110	CG	ASN	47	16.216	32.532	57.963	1.00	33.88	CPS5
ATOM	4111	OD1	ASN	47	15.427	31.588	57.896	1.00	34.99	CPS5
ATOM	4112	ND2	ASN	47	16.176	33.558	57.121	1.00	36.56	CPS5
ATOM	4113	C	ASN	47	18.944	31.440	57.513	1.00	31.05	CPS5
ATOM	4114	O	ASN	47	18.588	30.637	56.648	1.00	30.48	CPS5
ATOM	4115	N	GLU	48	19.888	32.358	57.311	1.00	28.97	CPS5
ATOM	4116	CA	GLU	48	20.588	32.468	56.031	1.00	29.63	CPS5
ATOM	4117	CB	GLU	48	21.570	33.640	56.061	1.00	31.86	CPS5
ATOM	4118	CG	GLU	48	20.921	34.975	56.372	1.00	37.62	CPS5
ATOM	4119	CD	GLU	48	21.936	36.092	56.540	1.00	40.25	CPS5
ATOM	4120	OE1	GLU	48	21.525	37.217	56.898	1.00	42.86	CPS5
ATOM	4121	OE2	GLU	48	23.141	35.845	56.313	1.00	41.40	CPS5
ATOM	4122	C	GLU	48	21.358	31.187	55.726	1.00	27.51	CPS5
ATOM	4123	O	GLU	48	21.281	30.644	54.622	1.00	26.82	CPS5
ATOM	4124	N	PHE	49	22.106	30.712	56.711	1.00	25.07	CPS5
ATOM	4125	CA	PHE	49	22.886	29.497	56.552	1.00	25.50	CPS5
ATOM	4126	CB	PHE	49	23.636	29.194	57.844	1.00	25.32	CPS5
ATOM	4127	CG	PHE	49	24.519	27.986	57.765	1.00	26.38	CPS5
ATOM	4128	CD1	PHE	49	25.798	28.077	57.233	1.00	27.15	CPS5
ATOM	4129	CD2	PHE	49	24.080	26.757	58.249	1.00	24.90	CPS5
ATOM	4130	CE1	PHE	49	26.640	26.954	57.189	1.00	28.06	CPS5
ATOM	4131	CE2	PHE	49	24.903	25.635	58.211	1.00	25.87	CPS5
ATOM	4132	CZ	PHE	49	26.195	25.736	57.678	1.00	26.35	CPS5
ATOM	4133	C	PHE	49	21.991	28.312	56.203	1.00	24.96	CPS5
ATOM	4134	O	PHE	49	22.255	27.581	55.248	1.00	24.24	CPS5
ATOM	4135	N	LEU	50	20.939	28.114	56.995	1.00	23.68	CPS5
ATOM	4136	CA	LEU	50	20.024	27.005	56.773	1.00	23.00	CPS5
ATOM	4137	CB	LEU	50	18.974	26.962	57.892	1.00	24.58	CPS5
ATOM	4138	CG	LEU	50	17.860	25.903	57.864	1.00	24.45	CPS5
ATOM	4139	CD1	LEU	50	18.431	24.483	57.785	1.00	24.94	CPS5
ATOM	4140	CD2	LEU	50	17.022	26.072	59.142	1.00	23.53	CPS5
ATOM	4141	C	LEU	50	19.349	27.082	55.403	1.00	22.61	CPS5
ATOM	4142	O	LEU	50	19.268	26.083	54.693	1.00	21.59	CPS5
ATOM	4143	N	ALA	51	18.865	28.260	55.021	1.00	21.89	CPS5
ATOM	4144	CA	ALA	51	18.213	28.390	53.723	1.00	21.84	CPS5
ATOM	4145	CB	ALA	51	17.637	29.799	53.556	1.00	21.05	CPS5
ATOM	4146	C	ALA	51	19.191	28.076	52.585	1.00	21.23	CPS5
ATOM	4147	O	ALA	51	18.813	27.458	51.587	1.00	21.60	CPS5
ATOM	4148	N	GLY	52	20.442	28.506	52.734	1.00	21.20	CPS5
ATOM	4149	CA	GLY	52	21.437	28.245	51.700	1.00	21.20	CPS5
ATOM	4150	C	GLY	52	21.769	26.767	51.563	1.00	22.06	CPS5
ATOM	4151	O	GLY	52	21.929	26.252	50.452	1.00	20.70	CPS5
ATOM	4152	N	ARG	53	21.888	26.074	52.693	1.00	21.88	CPS5
ATOM	4153	CA	ARG	53	22.188	24.645	52.659	1.00	21.58	CPS5
ATOM	4154	CB	ARG	53	22.565	24.152	54.065	1.00	23.65	CPS5
ATOM	4155	CG	ARG	53	24.066	24.127	54.329	1.00	27.20	CPS5
ATOM	4156	CD	ARG	53	24.751	25.409	53.912	1.00	30.18	CPS5
ATOM	4157	NE	ARG	53	26.181	25.365	54.194	1.00	32.58	CPS5
ATOM	4158	CZ	ARG	53	27.072	26.204	53.677	1.00	35.33	CPS5
ATOM	4159	NH1	ARG	53	26.690	27.163	52.836	1.00	37.77	CPS5
ATOM	4160	NH2	ARG	53	28.350	26.089	54.006	1.00	37.90	CPS5

FIG. 1A-73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ATOM   4161  C   ARG  53      20.976  23.890  52.125  1.00 21.40      CPS5
ATOM   4162  O   ARG  53      21.106  22.921  51.365  1.00 20.53      CPS5
ATOM   4163  N   PHE  54      19.795  24.341  52.528  1.00 19.73      CPS5
ATOM   4164  CA  PHE  54      18.548  23.745  52.070  1.00 19.35      CPS5
ATOM   4165  CB  PHE  54      17.364  24.482  52.724  1.00 19.38      CPS5
ATOM   4166  CG  PHE  54      16.023  23.926  52.353  1.00 20.72      CPS5
ATOM   4167  CD1 PHE  54      15.330  24.414  51.245  1.00 22.15      CPS5
ATOM   4168  CD2 PHE  54      15.448  22.903  53.107  1.00 21.41      CPS5
ATOM   4169  CE1 PHE  54      14.080  23.891  50.893  1.00 22.91      CPS5
ATOM   4170  CE2 PHE  54      14.196  22.371  52.762  1.00 22.41      CPS5
ATOM   4171  CZ  PHE  54      13.513  22.868  51.654  1.00 22.38      CPS5
ATOM   4172  C   PHE  54      18.484  23.873  50.537  1.00 19.62      CPS5
ATOM   4173  O   PHE  54      18.223  22.901  49.821  1.00 18.89      CPS5
ATOM   4174  N   ALA  55      18.736  25.082  50.046  1.00 19.98      CPS5
ATOM   4175  CA  ALA  55      18.690  25.348  48.608  1.00 19.92      CPS5
ATOM   4176  CB  ALA  55      18.930  26.839  48.347  1.00 18.81      CPS5
ATOM   4177  C   ALA  55      19.721  24.515  47.859  1.00 19.28      CPS5
ATOM   4178  O   ALA  55      19.442  23.972  46.788  1.00 19.25      CPS5
ATOM   4179  N   ALA  56      20.916  24.398  48.422  1.00 19.74      CPS5
ATOM   4180  CA  ALA  56      21.954  23.621  47.755  1.00 20.82      CPS5
ATOM   4181  CB  ALA  56      23.299  23.838  48.446  1.00 20.78      CPS5
ATOM   4182  C   ALA  56      21.622  22.130  47.693  1.00 20.48      CPS5
ATOM   4183  O   ALA  56      21.944  21.459  46.702  1.00 20.22      CPS5
ATOM   4184  N   LYS  57      20.993  21.600  48.746  1.00 19.44      CPS5
ATOM   4185  CA  LYS  57      20.642  20.187  48.754  1.00 19.12      CPS5
ATOM   4186  CB  LYS  57      20.336  19.718  50.191  1.00 18.95      CPS5
ATOM   4187  CG  LYS  57      21.571  19.809  51.077  1.00 18.78      CPS5
ATOM   4188  CD  LYS  57      21.395  19.116  52.429  1.00 22.43      CPS5
ATOM   4189  CE  LYS  57      22.575  19.458  53.329  1.00 22.68      CPS5
ATOM   4190  NZ  LYS  57      22.712  18.541  54.502  1.00 21.60      CPS5
ATOM   4191  C   LYS  57      19.465  19.937  47.821  1.00 20.77      CPS5
ATOM   4192  O   LYS  57      19.401  18.900  47.160  1.00 20.15      CPS5
ATOM   4193  N   GLU  58      18.535  20.885  47.757  1.00 19.45      CPS5
ATOM   4194  CA  GLU  58      17.410  20.738  46.845  1.00 21.16      CPS5
ATOM   4195  CB  GLU  58      16.409  21.887  47.020  1.00 21.14      CPS5
ATOM   4196  CG  GLU  58      15.520  21.769  48.247  1.00 25.24      CPS5
ATOM   4197  CD  GLU  58      14.558  20.605  48.153  1.00 29.18      CPS5
ATOM   4198  OE1 GLU  58      14.482  19.993  47.066  1.00 31.68      CPS5
ATOM   4199  OE2 GLU  58      13.875  20.305  49.156  1.00 29.87      CPS5
ATOM   4200  C   GLU  58      17.943  20.741  45.410  1.00 20.35      CPS5
ATOM   4201  O   GLU  58      17.543  19.908  44.590  1.00 20.00      CPS5
ATOM   4202  N   ALA  59      18.848  21.675  45.113  1.00 20.46      CPS5
ATOM   4203  CA  ALA  59      19.418  21.765  43.769  1.00 20.45      CPS5
ATOM   4204  CB  ALA  59      20.353  22.971  43.655  1.00 20.63      CPS5
ATOM   4205  C   ALA  59      20.175  20.489  43.436  1.00 20.79      CPS5
ATOM   4206  O   ALA  59      20.104  19.985  42.312  1.00 20.80      CPS5
ATOM   4207  N   PHE  60      20.916  19.965  44.404  1.00 19.71      CPS5
ATOM   4208  CA  PHE  60      21.643  18.730  44.153  1.00 19.50      CPS5
ATOM   4209  CB  PHE  60      22.511  18.349  45.361  1.00 20.28      CPS5
ATOM   4210  CG  PHE  60      23.252  17.057  45.172  1.00 22.22      CPS5
ATOM   4211  CD1 PHE  60      24.498  17.034  44.548  1.00 22.07      CPS5
ATOM   4212  CD2 PHE  60      22.657  15.850  45.538  1.00 23.50      CPS5
ATOM   4213  CE1 PHE  60      25.145  15.810  44.285  1.00 25.08      CPS5
ATOM   4214  CE2 PHE  60      23.287  14.629  45.282  1.00 26.22      CPS5
ATOM   4215  CZ  PHE  60      24.534  14.614  44.652  1.00 24.97      CPS5
ATOM   4216  C   PHE  60      20.665  17.588  43.857  1.00 19.97      CPS5
ATOM   4217  O   PHE  60      20.893  16.774  42.946  1.00 20.76      CPS5
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FIG. 1A-74

ATOM	4218	N	SER	61	19.575	17.530	44.615	1.00 19.93	CPS5
ATOM	4219	CA	SER	61	18.596	16.461	44.437	1.00 22.05	CPS5
ATOM	4220	CB	SER	61	17.542	16.505	45.550	1.00 21.89	CPS5
ATOM	4221	OG	SER	61	16.571	17.505	45.308	1.00 22.40	CPS5
ATOM	4222	C	SER	61	17.931	16.519	43.067	1.00 22.70	CPS5
ATOM	4223	O	SER	61	17.482	15.494	42.540	1.00 23.10	CPS5
ATOM	4224	N	LYS	62	17.874	17.716	42.487	1.00 21.75	CPS5
ATOM	4225	CA	LYS	62	17.292	17.888	41.158	1.00 22.11	CPS5
ATOM	4226	CB	LYS	62	16.914	19.349	40.932	1.00 23.25	CPS5
ATOM	4227	CG	LYS	62	15.636	19.790	41.661	1.00 26.97	CPS5
ATOM	4228	CD	LYS	62	15.515	21.316	41.597	1.00 29.60	CPS5
ATOM	4229	CE	LYS	62	14.085	21.787	41.383	1.00 33.49	CPS5
ATOM	4230	NZ	LYS	62	13.174	21.402	42.470	1.00 35.09	CPS5
ATOM	4231	C	LYS	62	18.290	17.431	40.095	1.00 22.61	CPS5
ATOM	4232	O	LYS	62	17.897	16.841	39.079	1.00 22.72	CPS5
ATOM	4233	N	ALA	63	19.577	17.695	40.333	1.00 21.05	CPS5
ATOM	4234	CA	ALA	63	20.627	17.283	39.408	1.00 21.93	CPS5
ATOM	4235	CB	ALA	63	21.965	17.909	39.801	1.00 21.40	CPS5
ATOM	4236	C	ALA	63	20.737	15.767	39.476	1.00 23.26	CPS5
ATOM	4237	O	ALA	63	21.006	15.113	38.473	1.00 22.70	CPS5
ATOM	4238	N	PHE	64	20.525	15.225	40.672	1.00 23.91	CPS5
ATOM	4239	CA	PHE	64	20.591	13.782	40.916	1.00 25.22	CPS5
ATOM	4240	CB	PHE	64	20.463	13.512	42.419	1.00 24.79	CPS5
ATOM	4241	CG	PHE	64	20.781	12.097	42.818	1.00 27.22	CPS5
ATOM	4242	CD1	PHE	64	22.094	11.642	42.822	1.00 28.51	CPS5
ATOM	4243	CD2	PHE	64	19.768	11.233	43.217	1.00 27.62	CPS5
ATOM	4244	CE1	PHE	64	22.398	10.343	43.224	1.00 30.62	CPS5
ATOM	4245	CE2	PHE	64	20.061	9.931	43.622	1.00 28.83	CPS5
ATOM	4246	CZ	PHE	64	21.377	9.489	43.625	1.00 28.53	CPS5
ATOM	4247	C	PHE	64	19.453	13.109	40.147	1.00 26.39	CPS5
ATOM	4248	O	PHE	64	19.554	11.941	39.766	1.00 28.07	CPS5
ATOM	4249	N	GLY	65	18.381	13.862	39.911	1.00 26.10	CPS5
ATOM	4250	CA	GLY	65	17.251	13.368	39.143	1.00 27.17	CPS5
ATOM	4251	C	GLY	65	16.088	12.768	39.905	1.00 28.46	CPS5
ATOM	4252	O	GLY	65	15.117	12.317	39.298	1.00 28.55	CPS5
ATOM	4253	N	THR	66	16.157	12.789	41.231	1.00 28.12	CPS5
ATOM	4254	CA	THR	66	15.099	12.191	42.037	1.00 29.33	CPS5
ATOM	4255	CB	THR	66	15.663	11.062	42.903	1.00 29.96	CPS5
ATOM	4256	OG1	THR	66	16.635	11.608	43.804	1.00 29.92	CPS5
ATOM	4257	CG2	THR	66	16.326	10.009	42.038	1.00 30.68	CPS5
ATOM	4258	C	THR	66	14.410	13.148	42.984	1.00 28.71	CPS5
ATOM	4259	O	THR	66	13.269	12.915	43.378	1.00 28.56	CPS5
ATOM	4260	N	GLY	67	15.098	14.227	43.343	1.00 27.58	CPS5
ATOM	4261	CA	GLY	67	14.530	15.150	44.305	1.00 27.06	CPS5
ATOM	4262	C	GLY	67	14.741	14.479	45.657	1.00 27.43	CPS5
ATOM	4263	O	GLY	67	15.278	13.367	45.712	1.00 26.28	CPS5
ATOM	4264	N	ILE	68	14.343	15.145	46.737	1.00 26.71	CPS5
ATOM	4265	CA	ILE	68	14.491	14.593	48.082	1.00 28.68	CPS5
ATOM	4266	CB	ILE	68	14.470	15.715	49.166	1.00 27.25	CPS5
ATOM	4267	CG2	ILE	68	14.574	15.098	50.569	1.00 27.25	CPS5
ATOM	4268	CG1	ILE	68	15.630	16.697	48.936	1.00 24.63	CPS5
ATOM	4269	CD1	ILE	68	17.030	16.084	49.112	1.00 23.40	CPS5
ATOM	4270	C	ILE	68	13.335	13.629	48.342	1.00 30.86	CPS5
ATOM	4271	O	ILE	68	12.167	13.982	48.169	1.00 31.01	CPS5
ATOM	4272	N	GLY	69	13.671	12.412	48.752	1.00 33.01	CPS5
ATOM	4273	CA	GLY	69	12.654	11.415	49.022	1.00 34.73	CPS5
ATOM	4274	C	GLY	69	13.291	10.115	49.470	1.00 36.57	CPS5

FIG. 1A-75

ATOM	4275	O	GLY	69	14.363	10.112	50.079	1.00 36.27	CPS5
ATOM	4276	N	ARG	70	12.653	8.997	49.152	1.00 38.18	CPS5
ATOM	4277	CA	ARG	70	13.203	7.724	49.579	1.00 39.66	CPS5
ATOM	4278	CB	ARG	70	12.137	6.627	49.493	1.00 43.12	CPS5
ATOM	4279	CG	ARG	70	11.182	6.661	50.696	1.00 47.23	CPS5
ATOM	4280	CD	ARG	70	11.972	6.780	52.019	1.00 49.65	CPS5
ATOM	4281	NE	ARG	70	11.469	7.858	52.870	1.00 51.86	CPS5
ATOM	4282	CZ	ARG	70	12.239	8.672	53.590	1.00 52.77	CPS5
ATOM	4283	NH1	ARG	70	13.558	8.540	53.569	1.00 53.05	CPS5
ATOM	4284	NH2	ARG	70	11.691	9.627	54.328	1.00 52.96	CPS5
ATOM	4285	C	ARG	70	14.468	7.317	48.855	1.00 37.80	CPS5
ATOM	4286	O	ARG	70	15.221	6.478	49.345	1.00 37.07	CPS5
ATOM	4287	N	GLN	71	14.726	7.926	47.703	1.00 36.29	CPS5
ATOM	4288	CA	GLN	71	15.932	7.598	46.959	1.00 35.22	CPS5
ATOM	4289	CB	GLN	71	15.707	7.778	45.453	1.00 36.48	CPS5
ATOM	4290	CG	GLN	71	14.534	6.985	44.889	1.00 38.95	CPS5
ATOM	4291	CD	GLN	71	14.402	7.129	43.379	1.00 40.20	CPS5
ATOM	4292	OE1	GLN	71	15.236	6.631	42.622	1.00 40.67	CPS5
ATOM	4293	NE2	GLN	71	13.355	7.827	42.937	1.00 40.72	CPS5
ATOM	4294	C	GLN	71	17.084	8.483	47.412	1.00 33.38	CPS5
ATOM	4295	O	GLN	71	18.248	8.110	47.276	1.00 33.43	CPS5
ATOM	4296	N	LEU	72	16.759	9.650	47.966	1.00 30.70	CPS5
ATOM	4297	CA	LEU	72	17.786	10.591	48.409	1.00 27.96	CPS5
ATOM	4298	CB	LEU	72	18.204	11.478	47.231	1.00 26.31	CPS5
ATOM	4299	CG	LEU	72	19.285	12.532	47.448	1.00 26.21	CPS5
ATOM	4300	CD1	LEU	72	20.626	11.867	47.673	1.00 27.19	CPS5
ATOM	4301	CD2	LEU	72	19.338	13.446	46.213	1.00 25.53	CPS5
ATOM	4302	C	LEU	72	17.279	11.469	49.556	1.00 27.62	CPS5
ATOM	4303	O	LEU	72	16.203	12.070	49.470	1.00 27.05	CPS5
ATOM	4304	N	SER	73	18.076	11.545	50.616	1.00 26.31	CPS5
ATOM	4305	CA	SER	73	17.735	12.323	51.805	1.00 25.42	CPS5
ATOM	4306	CB	SER	73	17.889	11.441	53.051	1.00 26.75	CPS5
ATOM	4307	OG	SER	73	17.970	12.228	54.231	1.00 27.96	CPS5
ATOM	4308	C	SER	73	18.633	13.539	51.965	1.00 24.08	CPS5
ATOM	4309	O	SER	73	19.733	13.581	51.419	1.00 23.91	CPS5
ATOM	4310	N	PHE	74	18.165	14.525	52.721	1.00 23.49	CPS5
ATOM	4311	CA	PHE	74	18.975	15.707	52.995	1.00 23.97	CPS5
ATOM	4312	CB	PHE	74	18.246	16.657	53.955	1.00 24.68	CPS5
ATOM	4313	CG	PHE	74	17.124	17.430	53.319	1.00 25.48	CPS5
ATOM	4314	CD1	PHE	74	17.392	18.421	52.371	1.00 26.10	CPS5
ATOM	4315	CD2	PHE	74	15.801	17.176	53.672	1.00 26.28	CPS5
ATOM	4316	CE1	PHE	74	16.347	19.151	51.786	1.00 25.75	CPS5
ATOM	4317	CE2	PHE	74	14.750	17.896	53.092	1.00 26.75	CPS5
ATOM	4318	CZ	PHE	74	15.028	18.886	52.148	1.00 25.31	CPS5
ATOM	4319	C	PHE	74	20.260	15.241	53.674	1.00 23.42	CPS5
ATOM	4320	O	PHE	74	21.334	15.804	53.459	1.00 23.30	CPS5
ATOM	4321	N	GLN	75	20.141	14.207	54.504	1.00 24.48	CPS5
ATOM	4322	CA	GLN	75	21.284	13.688	55.245	1.00 24.75	CPS5
ATOM	4323	CB	GLN	75	20.804	12.774	56.382	1.00 24.94	CPS5
ATOM	4324	CG	GLN	75	20.012	13.515	57.455	1.00 24.64	CPS5
ATOM	4325	CD	GLN	75	20.838	14.550	58.200	1.00 24.25	CPS5
ATOM	4326	OE1	GLN	75	20.304	15.559	58.674	1.00 28.14	CPS5
ATOM	4327	NE2	GLN	75	22.141	14.308	58.319	1.00 22.66	CPS5
ATOM	4328	C	GLN	75	22.316	12.958	54.390	1.00 26.96	CPS5
ATOM	4329	O	GLN	75	23.423	12.684	54.861	1.00 27.29	CPS5
ATOM	4330	N	ASP	76	21.965	12.651	53.144	1.00 27.28	CPS5
ATOM	4331	CA	ASP	76	22.906	11.976	52.245	1.00 28.96	CPS5

FIG. 1A-76

ATOM	4332	CB	ASP	76	22.171	11.187	51.157	1.00	28.71	CPS5
ATOM	4333	CG	ASP	76	21.422	10.002	51.695	1.00	30.19	CPS5
ATOM	4334	OD1	ASP	76	21.971	9.327	52.593	1.00	30.44	CPS5
ATOM	4335	OD2	ASP	76	20.296	9.733	51.211	1.00	30.21	CPS5
ATOM	4336	C	ASP	76	23.787	13.007	51.552	1.00	29.00	CPS5
ATOM	4337	O	ASP	76	24.738	12.652	50.856	1.00	30.49	CPS5
ATOM	4338	N	ILE	77	23.472	14.284	51.743	1.00	28.00	CPS5
ATOM	4339	CA	ILE	77	24.207	15.354	51.080	1.00	27.42	CPS5
ATOM	4340	CB	ILE	77	23.251	16.214	50.213	1.00	25.93	CPS5
ATOM	4341	CG2	ILE	77	24.067	17.152	49.328	1.00	26.70	CPS5
ATOM	4342	CG1	ILE	77	22.345	15.310	49.370	1.00	24.69	CPS5
ATOM	4343	CD1	ILE	77	21.036	15.971	48.941	1.00	25.15	CPS5
ATOM	4344	C	ILE	77	24.910	16.287	52.046	1.00	28.47	CPS5
ATOM	4345	O	ILE	77	24.287	16.853	52.943	1.00	29.75	CPS5
ATOM	4346	N	GLU	78	26.206	16.472	51.864	1.00	27.86	CPS5
ATOM	4347	CA	GLU	78	26.920	17.367	52.751	1.00	31.23	CPS5
ATOM	4348	CB	GLU	78	27.892	16.591	53.638	1.00	32.64	CPS5
ATOM	4349	CG	GLU	78	28.558	17.466	54.681	1.00	34.90	CPS5
ATOM	4350	CD	GLU	78	29.270	16.647	55.734	1.00	37.57	CPS5
ATOM	4351	OE1	GLU	78	30.334	16.072	55.425	1.00	38.97	CPS5
ATOM	4352	OE2	GLU	78	28.753	16.568	56.866	1.00	38.56	CPS5
ATOM	4353	C	GLU	78	27.676	18.468	52.042	1.00	31.73	CPS5
ATOM	4354	O	GLU	78	28.415	18.224	51.090	1.00	32.74	CPS5
ATOM	4355	N	ILE	79	27.481	19.691	52.508	1.00	32.96	CPS5
ATOM	4356	CA	ILE	79	28.177	20.821	51.932	1.00	35.99	CPS5
ATOM	4357	CB	ILE	79	27.265	22.044	51.818	1.00	36.51	CPS5
ATOM	4358	CG2	ILE	79	28.066	23.252	51.363	1.00	35.93	CPS5
ATOM	4359	CG1	ILE	79	26.129	21.738	50.842	1.00	37.54	CPS5
ATOM	4360	CD1	ILE	79	25.122	22.836	50.754	1.00	42.06	CPS5
ATOM	4361	C	ILE	79	29.342	21.145	52.842	1.00	38.38	CPS5
ATOM	4362	O	ILE	79	29.166	21.432	54.026	1.00	37.01	CPS5
ATOM	4363	N	ARG	80	30.543	21.075	52.290	1.00	42.32	CPS5
ATOM	4364	CA	ARG	80	31.729	21.371	53.070	1.00	46.50	CPS5
ATOM	4365	CB	ARG	80	32.690	20.180	53.091	1.00	46.70	CPS5
ATOM	4366	CG	ARG	80	32.116	18.913	53.670	1.00	48.52	CPS5
ATOM	4367	CD	ARG	80	33.151	17.798	53.687	1.00	49.02	CPS5
ATOM	4368	NE	ARG	80	32.519	16.508	53.945	1.00	50.86	CPS5
ATOM	4369	CZ	ARG	80	33.159	15.345	53.970	1.00	50.68	CPS5
ATOM	4370	NH1	ARG	80	34.465	15.303	53.757	1.00	50.94	CPS5
ATOM	4371	NH2	ARG	80	32.485	14.221	54.185	1.00	51.63	CPS5
ATOM	4372	C	ARG	80	32.444	22.545	52.459	1.00	48.41	CPS5
ATOM	4373	O	ARG	80	31.955	23.189	51.529	1.00	48.48	CPS5
ATOM	4374	N	LYS	81	33.616	22.820	53.003	1.00	51.83	CPS5
ATOM	4375	CA	LYS	81	34.448	23.892	52.507	1.00	54.26	CPS5
ATOM	4376	CB	LYS	81	34.388	25.099	53.445	1.00	55.70	CPS5
ATOM	4377	CG	LYS	81	32.994	25.704	53.578	1.00	58.10	CPS5
ATOM	4378	CD	LYS	81	33.014	26.958	54.439	1.00	59.69	CPS5
ATOM	4379	CE	LYS	81	31.606	27.467	54.730	1.00	61.09	CPS5
ATOM	4380	NZ	LYS	81	30.801	26.502	55.540	1.00	61.28	CPS5
ATOM	4381	C	LYS	81	35.847	23.307	52.459	1.00	54.90	CPS5
ATOM	4382	O	LYS	81	36.305	22.695	53.427	1.00	54.56	CPS5
ATOM	4383	N	ASP	82	36.504	23.452	51.314	1.00	55.76	CPS5
ATOM	4384	CA	ASP	82	37.855	22.940	51.151	1.00	56.67	CPS5
ATOM	4385	CB	ASP	82	38.281	23.026	49.683	1.00	56.75	CPS5
ATOM	4386	CG	ASP	82	37.874	24.337	49.031	1.00	56.88	CPS5
ATOM	4387	OD1	ASP	82	37.980	25.399	49.687	1.00	55.92	CPS5
ATOM	4388	OD2	ASP	82	37.457	24.301	47.853	1.00	57.36	CPS5

FIG. 1A-77

ATOM	4389	C	ASP	82	38.810	23.753	52.015	1.00 57.41	CPS5
ATOM	4390	O	ASP	82	38.377	24.523	52.874	1.00 56.93	CPS5
ATOM	4391	N	GLN	83	40.107	23.580	51.785	1.00 58.43	CPS5
ATOM	4392	CA	GLN	83	41.119	24.306	52.543	1.00 59.77	CPS5
ATOM	4393	CB	GLN	83	42.505	23.717	52.275	1.00 60.54	CPS5
ATOM	4394	CG	GLN	83	42.754	22.364	52.916	1.00 61.21	CPS5
ATOM	4395	CD	GLN	83	42.737	22.424	54.432	1.00 61.78	CPS5
ATOM	4396	OE1	GLN	83	41.674	22.447	55.054	1.00 62.24	CPS5
ATOM	4397	NE2	GLN	83	43.921	22.462	55.035	1.00 61.85	CPS5
ATOM	4398	C	GLN	83	41.117	25.793	52.189	1.00 60.23	CPS5
ATOM	4399	O	GLN	83	41.792	26.598	52.837	1.00 60.80	CPS5
ATOM	4400	N	ASN	84	40.359	26.153	51.157	1.00 59.89	CPS5
ATOM	4401	CA	ASN	84	40.268	27.543	50.730	1.00 59.63	CPS5
ATOM	4402	CB	ASN	84	40.373	27.636	49.207	1.00 60.60	CPS5
ATOM	4403	CG	ASN	84	41.707	27.140	48.685	1.00 61.37	CPS5
ATOM	4404	OD1	ASN	84	42.761	27.667	49.044	1.00 61.62	CPS5
ATOM	4405	ND2	ASN	84	41.669	26.120	47.834	1.00 61.98	CPS5
ATOM	4406	C	ASN	84	38.956	28.160	51.199	1.00 59.10	CPS5
ATOM	4407	O	ASN	84	38.731	29.361	51.037	1.00 59.66	CPS5
ATOM	4408	N	GLY	85	38.095	27.330	51.780	1.00 57.75	CPS5
ATOM	4409	CA	GLY	85	36.818	27.809	52.272	1.00 56.41	CPS5
ATOM	4410	C	GLY	85	35.731	27.794	51.213	1.00 55.75	CPS5
ATOM	4411	O	GLY	85	34.643	28.331	51.425	1.00 56.16	CPS5
ATOM	4412	N	LYS	86	36.022	27.180	50.070	1.00 54.26	CPS5
ATOM	4413	CA	LYS	86	35.058	27.107	48.978	1.00 52.12	CPS5
ATOM	4414	CB	LYS	86	35.775	26.812	47.657	1.00 53.72	CPS5
ATOM	4415	CG	LYS	86	34.948	27.105	46.406	1.00 55.30	CPS5
ATOM	4416	CD	LYS	86	34.812	28.604	46.171	1.00 56.46	CPS5
ATOM	4417	CE	LYS	86	34.012	28.910	44.905	1.00 56.79	CPS5
ATOM	4418	NZ	LYS	86	32.619	28.397	45.007	1.00 57.01	CPS5
ATOM	4419	C	LYS	86	34.057	25.999	49.279	1.00 49.78	CPS5
ATOM	4420	O	LYS	86	34.420	24.944	49.806	1.00 49.58	CPS5
ATOM	4421	N	PRO	87	32.777	26.222	48.952	1.00 47.09	CPS5
ATOM	4422	CD	PRO	87	32.162	27.432	48.380	1.00 46.07	CPS5
ATOM	4423	CA	PRO	87	31.764	25.198	49.214	1.00 44.34	CPS5
ATOM	4424	CB	PRO	87	30.469	25.995	49.177	1.00 44.60	CPS5
ATOM	4425	CG	PRO	87	30.745	26.967	48.074	1.00 45.82	CPS5
ATOM	4426	C	PRO	87	31.776	24.098	48.158	1.00 40.83	CPS5
ATOM	4427	O	PRO	87	31.837	24.382	46.961	1.00 40.94	CPS5
ATOM	4428	N	TYR	88	31.731	22.846	48.598	1.00 37.82	CPS5
ATOM	4429	CA	TYR	88	31.690	21.737	47.662	1.00 34.81	CPS5
ATOM	4430	CB	TYR	88	33.111	21.229	47.335	1.00 35.73	CPS5
ATOM	4431	CG	TYR	88	33.795	20.385	48.390	1.00 34.31	CPS5
ATOM	4432	CD1	TYR	88	33.648	19.002	48.399	1.00 34.27	CPS5
ATOM	4433	CE1	TYR	88	34.303	18.212	49.339	1.00 34.82	CPS5
ATOM	4434	CD2	TYR	88	34.615	20.966	49.354	1.00 35.40	CPS5
ATOM	4435	CE2	TYR	88	35.275	20.187	50.304	1.00 33.64	CPS5
ATOM	4436	CZ	TYR	88	35.112	18.812	50.290	1.00 35.08	CPS5
ATOM	4437	OH	TYR	88	35.730	18.028	51.239	1.00 35.18	CPS5
ATOM	4438	C	TYR	88	30.807	20.668	48.279	1.00 33.39	CPS5
ATOM	4439	O	TYR	88	30.627	20.633	49.497	1.00 32.83	CPS5
ATOM	4440	N	ILE	89	30.238	19.817	47.435	1.00 31.13	CPS5
ATOM	4441	CA	ILE	89	29.321	18.778	47.882	1.00 30.93	CPS5
ATOM	4442	CB	ILE	89	28.043	18.780	47.010	1.00 29.10	CPS5
ATOM	4443	CG2	ILE	89	27.189	17.547	47.303	1.00 27.98	CPS5
ATOM	4444	CG1	ILE	89	27.253	20.065	47.253	1.00 27.68	CPS5
ATOM	4445	CD1	ILE	89	26.041	20.215	46.364	1.00 27.97	CPS5

FIG. 1A-78

ATOM	4446	C	ILE	89	29.873	17.362	47.863	1.00 32.51	CPS5
ATOM	4447	O	ILE	89	30.637	16.987	46.973	1.00 31.03	CPS5
ATOM	4448	N	ILE	90	29.462	16.582	48.858	1.00 33.80	CPS5
ATOM	4449	CA	ILE	90	29.837	15.180	48.960	1.00 35.56	CPS5
ATOM	4450	CB	ILE	90	30.776	14.928	50.144	1.00 37.43	CPS5
ATOM	4451	CG2	ILE	90	30.959	13.418	50.359	1.00 37.12	CPS5
ATOM	4452	CG1	ILE	90	32.116	15.608	49.875	1.00 38.91	CPS5
ATOM	4453	CD1	ILE	90	33.093	15.508	51.006	1.00 42.45	CPS5
ATOM	4454	C	ILE	90	28.564	14.363	49.156	1.00 36.47	CPS5
ATOM	4455	O	ILE	90	27.782	14.624	50.076	1.00 35.64	CPS5
ATOM	4456	N	CYS	91	28.348	13.400	48.269	1.00 36.91	CPS5
ATOM	4457	CA	CYS	91	27.189	12.520	48.340	1.00 40.22	CPS5
ATOM	4458	CB	CYS	91	26.132	12.945	47.328	1.00 37.91	CPS5
ATOM	4459	SG	CYS	91	24.623	11.970	47.401	1.00 39.23	CPS5
ATOM	4460	C	CYS	91	27.643	11.094	48.035	1.00 42.93	CPS5
ATOM	4461	O	CYS	91	27.983	10.771	46.895	1.00 42.83	CPS5
ATOM	4462	N	THR	92	27.648	10.245	49.056	1.00 46.74	CPS5
ATOM	4463	CA	THR	92	28.070	8.858	48.881	1.00 50.26	CPS5
ATOM	4464	CB	THR	92	28.080	8.106	50.238	1.00 51.61	CPS5
ATOM	4465	OG1	THR	92	28.496	6.748	50.035	1.00 52.93	CPS5
ATOM	4466	CG2	THR	92	26.693	8.130	50.876	1.00 52.67	CPS5
ATOM	4467	C	THR	92	27.175	8.110	47.890	1.00 51.62	CPS5
ATOM	4468	O	THR	92	27.656	7.285	47.108	1.00 51.98	CPS5
ATOM	4469	N	LYS	93	25.879	8.413	47.914	1.00 52.57	CPS5
ATOM	4470	CA	LYS	93	24.918	7.769	47.020	1.00 53.74	CPS5
ATOM	4471	CB	LYS	93	23.503	8.289	47.296	1.00 54.52	CPS5
ATOM	4472	CG	LYS	93	23.041	8.147	48.742	1.00 56.49	CPS5
ATOM	4473	CD	LYS	93	22.706	6.708	49.101	1.00 57.62	CPS5
ATOM	4474	CE	LYS	93	21.372	6.279	48.501	1.00 58.57	CPS5
ATOM	4475	NZ	LYS	93	20.218	7.009	49.109	1.00 59.31	CPS5
ATOM	4476	C	LYS	93	25.262	8.027	45.556	1.00 53.90	CPS5
ATOM	4477	O	LYS	93	24.681	7.419	44.656	1.00 54.01	CPS5
ATOM	4478	N	LEU	94	26.213	8.926	45.322	1.00 53.85	CPS5
ATOM	4479	CA	LEU	94	26.605	9.283	43.967	1.00 54.05	CPS5
ATOM	4480	CB	LEU	94	26.967	10.770	43.904	1.00 54.55	CPS5
ATOM	4481	CG	LEU	94	26.620	11.562	42.640	1.00 54.80	CPS5
ATOM	4482	CD1	LEU	94	27.225	12.951	42.751	1.00 54.69	CPS5
ATOM	4483	CD2	LEU	94	27.143	10.857	41.405	1.00 55.41	CPS5
ATOM	4484	C	LEU	94	27.780	8.466	43.452	1.00 54.05	CPS5
ATOM	4485	O	LEU	94	28.797	8.322	44.130	1.00 54.64	CPS5
ATOM	4486	N	SER	95	27.626	7.934	42.246	1.00 53.47	CPS5
ATOM	4487	CA	SER	95	28.673	7.155	41.603	1.00 53.51	CPS5
ATOM	4488	CB	SER	95	28.131	6.559	40.299	1.00 54.31	CPS5
ATOM	4489	OG	SER	95	29.138	5.881	39.574	1.00 56.70	CPS5
ATOM	4490	C	SER	95	29.812	8.134	41.315	1.00 52.59	CPS5
ATOM	4491	O	SER	95	29.589	9.345	41.279	1.00 53.14	CPS5
ATOM	4492	N	PRO	96	31.046	7.636	41.121	1.00 51.05	CPS5
ATOM	4493	CD	PRO	96	31.511	6.248	40.992	1.00 51.64	CPS5
ATOM	4494	CA	PRO	96	32.140	8.572	40.843	1.00 49.02	CPS5
ATOM	4495	CB	PRO	96	33.252	7.670	40.285	1.00 50.01	CPS5
ATOM	4496	CG	PRO	96	32.537	6.387	39.898	1.00 51.26	CPS5
ATOM	4497	C	PRO	96	31.731	9.680	39.878	1.00 47.02	CPS5
ATOM	4498	O	PRO	96	31.238	9.425	38.775	1.00 46.21	CPS5
ATOM	4499	N	ALA	97	31.931	10.917	40.313	1.00 44.30	CPS5
ATOM	4500	CA	ALA	97	31.566	12.063	39.499	1.00 41.77	CPS5
ATOM	4501	CB	ALA	97	30.055	12.176	39.425	1.00 40.64	CPS5
ATOM	4502	C	ALA	97	32.140	13.342	40.071	1.00 40.33	CPS5

FIG. 1A-79

ATOM	4503	O	ALA	97	32.593	13.382	41.216	1.00	40.58	CPS5
ATOM	4504	N	ALA	98	32.121	14.387	39.256	1.00	37.31	CPS5
ATOM	4505	CA	ALA	98	32.597	15.688	39.676	1.00	34.75	CPS5
ATOM	4506	CB	ALA	98	33.398	16.340	38.561	1.00	35.64	CPS5
ATOM	4507	C	ALA	98	31.308	16.463	39.941	1.00	32.51	CPS5
ATOM	4508	O	ALA	98	30.407	16.478	39.107	1.00	31.77	CPS5
ATOM	4509	N	VAL	99	31.204	17.061	41.119	1.00	29.38	CPS5
ATOM	4510	CA	VAL	99	30.017	17.823	41.476	1.00	26.77	CPS5
ATOM	4511	CB	VAL	99	29.409	17.320	42.808	1.00	26.38	CPS5
ATOM	4512	CG1	VAL	99	28.128	18.089	43.132	1.00	25.70	CPS5
ATOM	4513	CG2	VAL	99	29.110	15.821	42.708	1.00	26.03	CPS5
ATOM	4514	C	VAL	99	30.460	19.270	41.632	1.00	25.29	CPS5
ATOM	4515	O	VAL	99	31.518	19.541	42.192	1.00	24.54	CPS5
ATOM	4516	N	HIS	100	29.655	20.190	41.113	1.00	23.97	CPS5
ATOM	4517	CA	HIS	100	29.949	21.615	41.203	1.00	23.10	CPS5
ATOM	4518	CB	HIS	100	30.225	22.176	39.819	1.00	24.86	CPS5
ATOM	4519	CG	HIS	100	31.328	21.468	39.105	1.00	26.57	CPS5
ATOM	4520	CD2	HIS	100	31.297	20.480	38.181	1.00	27.57	CPS5
ATOM	4521	ND1	HIS	100	32.660	21.719	39.358	1.00	28.54	CPS5
ATOM	4522	CE1	HIS	100	33.403	20.915	38.618	1.00	28.60	CPS5
ATOM	4523	NE2	HIS	100	32.599	20.155	37.894	1.00	28.27	CPS5
ATOM	4524	C	HIS	100	28.728	22.293	41.791	1.00	22.08	CPS5
ATOM	4525	O	HIS	100	27.602	21.917	41.475	1.00	21.49	CPS5
ATOM	4526	N	VAL	101	28.944	23.288	42.640	1.00	20.70	CPS5
ATOM	4527	CA	VAL	101	27.823	23.980	43.254	1.00	20.32	CPS5
ATOM	4528	CB	VAL	101	27.503	23.372	44.672	1.00	21.79	CPS5
ATOM	4529	CG1	VAL	101	28.687	23.560	45.614	1.00	21.73	CPS5
ATOM	4530	CG2	VAL	101	26.253	24.021	45.281	1.00	20.57	CPS5
ATOM	4531	C	VAL	101	28.137	25.462	43.385	1.00	20.62	CPS5
ATOM	4532	O	VAL	101	29.299	25.863	43.370	1.00	20.26	CPS5
ATOM	4533	N	SER	102	27.091	26.281	43.448	1.00	18.85	CPS5
ATOM	4534	CA	SER	102	27.256	27.709	43.670	1.00	18.73	CPS5
ATOM	4535	CB	SER	102	27.292	28.509	42.363	1.00	19.66	CPS5
ATOM	4536	OG	SER	102	27.474	29.886	42.685	1.00	19.70	CPS5
ATOM	4537	C	SER	102	26.037	28.118	44.489	1.00	19.25	CPS5
ATOM	4538	O	SER	102	24.931	27.684	44.200	1.00	17.98	CPS5
ATOM	4539	N	ILE	103	26.246	28.928	45.520	1.00	19.07	CPS5
ATOM	4540	CA	ILE	103	25.153	29.374	46.377	1.00	20.39	CPS5
ATOM	4541	CB	ILE	103	25.347	28.876	47.833	1.00	22.16	CPS5
ATOM	4542	CG2	ILE	103	24.216	29.404	48.736	1.00	22.36	CPS5
ATOM	4543	CG1	ILE	103	25.363	27.350	47.865	1.00	21.89	CPS5
ATOM	4544	CD1	ILE	103	25.821	26.762	49.214	1.00	24.06	CPS5
ATOM	4545	C	ILE	103	25.157	30.892	46.358	1.00	21.36	CPS5
ATOM	4546	O	ILE	103	26.225	31.512	46.304	1.00	21.80	CPS5
ATOM	4547	N	THR	104	23.968	31.489	46.374	1.00	21.34	CPS5
ATOM	4548	CA	THR	104	23.839	32.938	46.347	1.00	22.25	CPS5
ATOM	4549	CB	THR	104	23.591	33.450	44.901	1.00	24.00	CPS5
ATOM	4550	OG1	THR	104	23.661	34.887	44.864	1.00	24.60	CPS5
ATOM	4551	CG2	THR	104	22.235	32.998	44.399	1.00	23.88	CPS5
ATOM	4552	C	THR	104	22.705	33.376	47.276	1.00	23.21	CPS5
ATOM	4553	O	THR	104	21.831	32.579	47.641	1.00	21.95	CPS5
ATOM	4554	N	HIS	105	22.728	34.645	47.664	1.00	24.23	CPS5
ATOM	4555	CA	HIS	105	21.723	35.181	48.578	1.00	26.22	CPS5
ATOM	4556	CB	HIS	105	22.287	35.276	50.003	1.00	27.67	CPS5
ATOM	4557	CG	HIS	105	22.810	33.988	50.555	1.00	30.95	CPS5
ATOM	4558	CD2	HIS	105	24.036	33.417	50.475	1.00	32.56	CPS5
ATOM	4559	ND1	HIS	105	22.046	33.146	51.333	1.00	32.46	CPS5

FIG. 1A-80

ATOM	4560	CE1	HIS	105	22.777	32.114	51.713	1.00 32.44	CPS5
ATOM	4561	NE2	HIS	105	23.990	32.253	51.206	1.00 32.77	CPS5
ATOM	4562	C	HIS	105	21.291	36.596	48.218	1.00 25.94	CPS5
ATOM	4563	O	HIS	105	22.037	37.344	47.584	1.00 25.81	CPS5
ATOM	4564	N	THR	106	20.077	36.944	48.630	1.00 25.98	CPS5
ATOM	4565	CA	THR	106	19.569	38.305	48.498	1.00 26.59	CPS5
ATOM	4566	CB	THR	106	18.474	38.498	47.436	1.00 26.91	CPS5
ATOM	4567	OG1	THR	106	17.305	37.771	47.813	1.00 26.20	CPS5
ATOM	4568	CG2	THR	106	18.963	38.070	46.062	1.00 25.16	CPS5
ATOM	4569	C	THR	106	18.946	38.516	49.870	1.00 27.65	CPS5
ATOM	4570	O	THR	106	19.024	37.638	50.733	1.00 26.71	CPS5
ATOM	4571	N	LYS	107	18.330	39.667	50.086	1.00 28.18	CPS5
ATOM	4572	CA	LYS	107	17.716	39.938	51.377	1.00 29.86	CPS5
ATOM	4573	CB	LYS	107	17.103	41.345	51.366	1.00 32.21	CPS5
ATOM	4574	CG	LYS	107	16.495	41.791	52.690	1.00 36.65	CPS5
ATOM	4575	CD	LYS	107	15.848	43.171	52.540	1.00 40.32	CPS5
ATOM	4576	CE	LYS	107	15.282	43.682	53.860	1.00 42.28	CPS5
ATOM	4577	NZ	LYS	107	14.641	45.026	53.709	1.00 45.02	CPS5
ATOM	4578	C	LYS	107	16.645	38.910	51.754	1.00 29.02	CPS5
ATOM	4579	O	LYS	107	16.576	38.484	52.908	1.00 29.89	CPS5
ATOM	4580	N	GLU	108	15.830	38.495	50.785	1.00 27.24	CPS5
ATOM	4581	CA	GLU	108	14.733	37.568	51.063	1.00 26.97	CPS5
ATOM	4582	CB	GLU	108	13.428	38.156	50.525	1.00 29.17	CPS5
ATOM	4583	CG	GLU	108	13.129	39.552	51.030	1.00 35.90	CPS5
ATOM	4584	CD	GLU	108	11.758	40.043	50.612	1.00 40.16	CPS5
ATOM	4585	OE1	GLU	108	11.459	40.044	49.397	1.00 43.68	CPS5
ATOM	4586	OE2	GLU	108	10.975	40.436	51.505	1.00 44.69	CPS5
ATOM	4587	C	GLU	108	14.855	36.149	50.527	1.00 24.76	CPS5
ATOM	4588	O	GLU	108	14.007	35.300	50.823	1.00 23.74	CPS5
ATOM	4589	N	TYR	109	15.889	35.888	49.738	1.00 23.62	CPS5
ATOM	4590	CA	TYR	109	16.045	34.564	49.137	1.00 23.16	CPS5
ATOM	4591	CB	TYR	109	15.695	34.627	47.645	1.00 23.09	CPS5
ATOM	4592	CG	TYR	109	14.286	35.052	47.352	1.00 23.49	CPS5
ATOM	4593	CD1	TYR	109	13.243	34.135	47.403	1.00 24.28	CPS5
ATOM	4594	CE1	TYR	109	11.931	34.529	47.199	1.00 24.85	CPS5
ATOM	4595	CD2	TYR	109	13.982	36.390	47.080	1.00 26.20	CPS5
ATOM	4596	CE2	TYR	109	12.667	36.797	46.874	1.00 25.83	CPS5
ATOM	4597	CZ	TYR	109	11.648	35.861	46.937	1.00 25.55	CPS5
ATOM	4598	OH	TYR	109	10.341	36.243	46.769	1.00 26.59	CPS5
ATOM	4599	C	TYR	109	17.438	33.976	49.230	1.00 22.83	CPS5
ATOM	4600	O	TYR	109	18.421	34.691	49.403	1.00 23.71	CPS5
ATOM	4601	N	ALA	110	17.490	32.650	49.128	1.00 21.41	CPS5
ATOM	4602	CA	ALA	110	18.744	31.912	49.055	1.00 21.16	CPS5
ATOM	4603	CB	ALA	110	18.924	30.988	50.258	1.00 20.41	CPS5
ATOM	4604	C	ALA	110	18.536	31.089	47.785	1.00 20.71	CPS5
ATOM	4605	O	ALA	110	17.415	30.635	47.508	1.00 21.39	CPS5
ATOM	4606	N	ALA	111	19.589	30.915	46.991	1.00 19.32	CPS5
ATOM	4607	CA	ALA	111	19.467	30.131	45.771	1.00 18.05	CPS5
ATOM	4608	CB	ALA	111	19.215	31.033	44.575	1.00 18.98	CPS5
ATOM	4609	C	ALA	111	20.734	29.344	45.550	1.00 19.39	CPS5
ATOM	4610	O	ALA	111	21.800	29.707	46.050	1.00 18.83	CPS5
ATOM	4611	N	ALA	112	20.623	28.269	44.786	1.00 18.45	CPS5
ATOM	4612	CA	ALA	112	21.784	27.451	44.508	1.00 19.52	CPS5
ATOM	4613	CB	ALA	112	22.008	26.481	45.655	1.00 19.65	CPS5
ATOM	4614	C	ALA	112	21.617	26.679	43.212	1.00 18.81	CPS5
ATOM	4615	O	ALA	112	20.502	26.442	42.764	1.00 17.20	CPS5
ATOM	4616	N	GLN	113	22.733	26.311	42.599	1.00 19.37	CPS5

FIG. 1A-81

ATOM	4617	CA	GLN	113	22.663	25.499	41.400	1.00	20.01	CPS5
ATOM	4618	CB	GLN	113	22.890	26.321	40.135	1.00	23.47	CPS5
ATOM	4619	CG	GLN	113	24.249	26.942	40.040	1.00	26.43	CPS5
ATOM	4620	CD	GLN	113	24.463	27.640	38.705	1.00	30.41	CPS5
ATOM	4621	OE1	GLN	113	25.506	28.234	38.467	1.00	29.83	CPS5
ATOM	4622	NE2	GLN	113	23.466	27.567	37.831	1.00	33.75	CPS5
ATOM	4623	C	GLN	113	23.735	24.439	41.518	1.00	19.96	CPS5
ATOM	4624	O	GLN	113	24.753	24.633	42.177	1.00	19.44	CPS5
ATOM	4625	N	VAL	114	23.504	23.312	40.869	1.00	19.35	CPS5
ATOM	4626	CA	VAL	114	24.462	22.221	40.924	1.00	19.11	CPS5
ATOM	4627	CB	VAL	114	23.960	21.111	41.897	1.00	18.72	CPS5
ATOM	4628	CG1	VAL	114	24.791	19.828	41.721	1.00	20.30	CPS5
ATOM	4629	CG2	VAL	114	24.043	21.603	43.344	1.00	20.16	CPS5
ATOM	4630	C	VAL	114	24.589	21.611	39.538	1.00	19.40	CPS5
ATOM	4631	O	VAL	114	23.618	21.590	38.781	1.00	19.86	CPS5
ATOM	4632	N	VAL	115	25.792	21.159	39.201	1.00	19.59	CPS5
ATOM	4633	CA	VAL	115	26.017	20.436	37.956	1.00	19.26	CPS5
ATOM	4634	CB	VAL	115	26.879	21.202	36.928	1.00	20.70	CPS5
ATOM	4635	CG1	VAL	115	27.182	20.280	35.725	1.00	19.97	CPS5
ATOM	4636	CG2	VAL	115	26.131	22.443	36.433	1.00	19.15	CPS5
ATOM	4637	C	VAL	115	26.780	19.172	38.359	1.00	22.16	CPS5
ATOM	4638	O	VAL	115	27.765	19.248	39.092	1.00	21.19	CPS5
ATOM	4639	N	ILE	116	26.291	18.018	37.920	1.00	23.19	CPS5
ATOM	4640	CA	ILE	116	26.965	16.749	38.201	1.00	25.23	CPS5
ATOM	4641	CB	ILE	116	25.983	15.681	38.761	1.00	24.21	CPS5
ATOM	4642	CG2	ILE	116	26.717	14.347	38.952	1.00	24.03	CPS5
ATOM	4643	CG1	ILE	116	25.401	16.139	40.106	1.00	24.21	CPS5
ATOM	4644	CD1	ILE	116	24.294	15.209	40.635	1.00	22.70	CPS5
ATOM	4645	C	ILE	116	27.521	16.243	36.866	1.00	26.72	CPS5
ATOM	4646	O	ILE	116	26.788	16.165	35.881	1.00	25.85	CPS5
ATOM	4647	N	GLU	117	28.809	15.914	36.835	1.00	30.40	CPS5
ATOM	4648	CA	GLU	117	29.447	15.401	35.615	1.00	35.53	CPS5
ATOM	4649	CB	GLU	117	30.792	16.064	35.352	1.00	36.89	CPS5
ATOM	4650	CG	GLU	117	30.816	17.554	35.274	1.00	39.07	CPS5
ATOM	4651	CD	GLU	117	32.168	18.036	34.808	1.00	39.75	CPS5
ATOM	4652	OE1	GLU	117	32.457	17.877	33.605	1.00	40.89	CPS5
ATOM	4653	OE2	GLU	117	32.948	18.547	35.641	1.00	40.65	CPS5
ATOM	4654	C	GLU	117	29.735	13.915	35.771	1.00	38.76	CPS5
ATOM	4655	O	GLU	117	30.317	13.501	36.782	1.00	38.92	CPS5
ATOM	4656	N	ALA	118	29.364	13.131	34.761	1.00	41.50	CPS5
ATOM	4657	CA	ALA	118	29.596	11.689	34.784	1.00	44.75	CPS5
ATOM	4658	CB	ALA	118	29.047	11.049	33.508	1.00	45.12	CPS5
ATOM	4659	C	ALA	118	31.095	11.422	34.899	1.00	46.14	CPS5
ATOM	4660	OT1	ALA	118	31.885	12.266	34.413	1.00	46.30	CPS5
ATOM	4661	OT2	ALA	118	31.460	10.367	35.466	1.00	48.44	CPS5
ATOM	4662	C	GLY	1	34.929	20.508	32.382	1.00	33.16	CPS6
ATOM	4663	O	GLY	1	35.455	21.500	31.885	1.00	34.15	CPS6
ATOM	4664	N	GLY	1	36.363	18.424	32.401	1.00	38.41	CPS6
ATOM	4665	CA	GLY	1	35.171	19.118	31.815	1.00	34.91	CPS6
ATOM	4666	N	ILE	2	34.133	20.587	33.435	1.00	30.97	CPS6
ATOM	4667	CA	ILE	2	33.824	21.875	34.039	1.00	28.64	CPS6
ATOM	4668	CB	ILE	2	32.405	21.855	34.627	1.00	27.89	CPS6
ATOM	4669	CG2	ILE	2	32.168	23.101	35.474	1.00	27.12	CPS6
ATOM	4670	CG1	ILE	2	31.386	21.726	33.490	1.00	28.03	CPS6
ATOM	4671	CD1	ILE	2	29.965	21.432	33.954	1.00	28.46	CPS6
ATOM	4672	C	ILE	2	34.810	22.262	35.134	1.00	28.03	CPS6
ATOM	4673	O	ILE	2	35.117	21.463	36.011	1.00	27.12	CPS6

FIG. 1A-82

ATOM	4674	N	TYR	3	35.305	23.492	35.080	1.00	26.59	CPS6
ATOM	4675	CA	TYR	3	36.234	23.970	36.101	1.00	26.25	CPS6
ATOM	4676	CB	TYR	3	37.102	25.091	35.540	1.00	27.53	CPS6
ATOM	4677	CG	TYR	3	38.027	25.703	36.570	1.00	31.25	CPS6
ATOM	4678	CD1	TYR	3	39.171	25.027	36.999	1.00	32.43	CPS6
ATOM	4679	CE1	TYR	3	40.006	25.568	37.978	1.00	35.68	CPS6
ATOM	4680	CD2	TYR	3	37.738	26.937	37.146	1.00	31.55	CPS6
ATOM	4681	CE2	TYR	3	38.563	27.489	38.126	1.00	35.40	CPS6
ATOM	4682	CZ	TYR	3	39.697	26.800	38.537	1.00	36.39	CPS6
ATOM	4683	OH	TYR	3	40.525	27.355	39.488	1.00	39.51	CPS6
ATOM	4684	C	TYR	3	35.451	24.482	37.316	1.00	25.81	CPS6
ATOM	4685	O	TYR	3	35.762	24.145	38.469	1.00	24.16	CPS6
ATOM	4686	N	GLY	4	34.437	25.301	37.058	1.00	22.42	CPS6
ATOM	4687	CA	GLY	4	33.630	25.823	38.147	1.00	22.32	CPS6
ATOM	4688	C	GLY	4	32.365	26.494	37.642	1.00	20.34	CPS6
ATOM	4689	O	GLY	4	32.280	26.799	36.461	1.00	19.69	CPS6
ATOM	4690	N	ILE	5	31.389	26.704	38.525	1.00	20.01	CPS6
ATOM	4691	CA	ILE	5	30.140	27.366	38.143	1.00	20.35	CPS6
ATOM	4692	CB	ILE	5	28.947	26.382	38.097	1.00	20.14	CPS6
ATOM	4693	CG2	ILE	5	29.291	25.224	37.159	1.00	19.26	CPS6
ATOM	4694	CG1	ILE	5	28.600	25.876	39.507	1.00	19.61	CPS6
ATOM	4695	CD1	ILE	5	27.418	24.871	39.535	1.00	21.63	CPS6
ATOM	4696	C	ILE	5	29.832	28.481	39.119	1.00	20.43	CPS6
ATOM	4697	O	ILE	5	30.337	28.505	40.242	1.00	20.18	CPS6
ATOM	4698	N	GLY	6	29.009	29.426	38.686	1.00	19.58	CPS6
ATOM	4699	CA	GLY	6	28.681	30.532	39.560	1.00	19.69	CPS6
ATOM	4700	C	GLY	6	27.279	31.023	39.287	1.00	19.25	CPS6
ATOM	4701	O	GLY	6	26.842	31.080	38.135	1.00	17.69	CPS6
ATOM	4702	N	LEU	7	26.581	31.374	40.358	1.00	19.31	CPS6
ATOM	4703	CA	LEU	7	25.214	31.865	40.262	1.00	20.65	CPS6
ATOM	4704	CB	LEU	7	24.249	30.808	40.811	1.00	20.48	CPS6
ATOM	4705	CG	LEU	7	22.781	31.222	40.967	1.00	21.08	CPS6
ATOM	4706	CD1	LEU	7	22.175	31.455	39.576	1.00	22.40	CPS6
ATOM	4707	CD2	LEU	7	22.017	30.132	41.724	1.00	21.05	CPS6
ATOM	4708	C	LEU	7	25.108	33.114	41.116	1.00	20.36	CPS6
ATOM	4709	O	LEU	7	25.687	33.180	42.193	1.00	21.58	CPS6
ATOM	4710	N	ASP	8	24.387	34.114	40.631	1.00	20.16	CPS6
ATOM	4711	CA	ASP	8	24.188	35.310	41.423	1.00	21.86	CPS6
ATOM	4712	CB	ASP	8	25.261	36.368	41.151	1.00	23.79	CPS6
ATOM	4713	CG	ASP	8	25.018	37.637	41.948	1.00	26.23	CPS6
ATOM	4714	OD1	ASP	8	24.287	38.523	41.462	1.00	26.66	CPS6
ATOM	4715	OD2	ASP	8	25.523	37.725	43.081	1.00	27.19	CPS6
ATOM	4716	C	ASP	8	22.838	35.935	41.173	1.00	21.30	CPS6
ATOM	4717	O	ASP	8	22.379	35.977	40.041	1.00	20.01	CPS6
ATOM	4718	N	ILE	9	22.184	36.384	42.242	1.00	20.98	CPS6
ATOM	4719	CA	ILE	9	20.911	37.081	42.099	1.00	20.91	CPS6
ATOM	4720	CB	ILE	9	19.733	36.347	42.787	1.00	21.99	CPS6
ATOM	4721	CG2	ILE	9	18.456	37.172	42.639	1.00	20.05	CPS6
ATOM	4722	CG1	ILE	9	19.543	34.963	42.159	1.00	20.50	CPS6
ATOM	4723	CD1	ILE	9	18.405	34.165	42.754	1.00	21.55	CPS6
ATOM	4724	C	ILE	9	21.160	38.402	42.803	1.00	22.15	CPS6
ATOM	4725	O	ILE	9	21.683	38.420	43.918	1.00	23.20	CPS6
ATOM	4726	N	THR	10	20.813	39.505	42.148	1.00	24.06	CPS6
ATOM	4727	CA	THR	10	21.033	40.826	42.722	1.00	25.03	CPS6
ATOM	4728	CB	THR	10	22.125	41.578	41.915	1.00	27.35	CPS6
ATOM	4729	OG1	THR	10	23.375	40.882	42.054	1.00	27.27	CPS6
ATOM	4730	CG2	THR	10	22.299	43.006	42.413	1.00	28.83	CPS6

FIG. 1A-83

ATOM	4731	C	THR	10	19.734	41.626	42.734	1.00 25.30	CPS6
ATOM	4732	O	THR	10	18.978	41.620	41.762	1.00 24.09	CPS6
ATOM	4733	N	GLU	11	19.475	42.290	43.857	1.00 24.60	CPS6
ATOM	4734	CA	GLU	11	18.278	43.112	44.025	1.00 25.85	CPS6
ATOM	4735	CB	GLU	11	18.012	43.306	45.525	1.00 26.85	CPS6
ATOM	4736	CG	GLU	11	16.635	43.843	45.872	1.00 30.57	CPS6
ATOM	4737	CD	GLU	11	16.506	44.224	47.342	1.00 33.54	CPS6
ATOM	4738	OE1	GLU	11	17.435	43.928	48.136	1.00 34.46	CPS6
ATOM	4739	OE2	GLU	11	15.469	44.821	47.701	1.00 34.21	CPS6
ATOM	4740	C	GLU	11	18.533	44.467	43.354	1.00 25.21	CPS6
ATOM	4741	O	GLU	11	19.499	45.150	43.694	1.00 26.16	CPS6
ATOM	4742	N	LEU	12	17.687	44.855	42.402	1.00 26.01	CPS6
ATOM	4743	CA	LEU	12	17.870	46.138	41.713	1.00 28.08	CPS6
ATOM	4744	CB	LEU	12	16.733	46.381	40.707	1.00 28.52	CPS6
ATOM	4745	CG	LEU	12	16.880	45.889	39.264	1.00 31.49	CPS6
ATOM	4746	CD1	LEU	12	17.467	44.495	39.234	1.00 30.71	CPS6
ATOM	4747	CD2	LEU	12	15.530	45.921	38.573	1.00 32.17	CPS6
ATOM	4748	C	LEU	12	17.926	47.301	42.708	1.00 29.26	CPS6
ATOM	4749	O	LEU	12	18.732	48.223	42.553	1.00 29.98	CPS6
ATOM	4750	N	ALA	13	17.067	47.258	43.725	1.00 29.78	CPS6
ATOM	4751	CA	ALA	13	17.027	48.315	44.733	1.00 30.29	CPS6
ATOM	4752	CB	ALA	13	15.901	48.042	45.741	1.00 31.01	CPS6
ATOM	4753	C	ALA	13	18.364	48.447	45.460	1.00 31.44	CPS6
ATOM	4754	O	ALA	13	18.774	49.551	45.825	1.00 31.56	CPS6
ATOM	4755	N	ARG	14	19.048	47.327	45.669	1.00 32.19	CPS6
ATOM	4756	CA	ARG	14	20.338	47.357	46.352	1.00 32.76	CPS6
ATOM	4757	CB	ARG	14	20.745	45.940	46.768	1.00 35.66	CPS6
ATOM	4758	CG	ARG	14	22.097	45.852	47.437	1.00 39.95	CPS6
ATOM	4759	CD	ARG	14	22.314	44.493	48.078	1.00 42.90	CPS6
ATOM	4760	NE	ARG	14	23.727	44.261	48.363	1.00 46.95	CPS6
ATOM	4761	CZ	ARG	14	24.577	43.675	47.524	1.00 48.91	CPS6
ATOM	4762	NH1	ARG	14	24.163	43.247	46.338	1.00 50.22	CPS6
ATOM	4763	NH2	ARG	14	25.850	43.523	47.868	1.00 50.46	CPS6
ATOM	4764	C	ARG	14	21.415	48.002	45.469	1.00 32.36	CPS6
ATOM	4765	O	ARG	14	22.268	48.747	45.961	1.00 31.82	CPS6
ATOM	4766	N	ILE	15	21.381	47.719	44.171	1.00 31.44	CPS6
ATOM	4767	CA	ILE	15	22.337	48.326	43.247	1.00 31.99	CPS6
ATOM	4768	CB	ILE	15	22.153	47.777	41.817	1.00 32.07	CPS6
ATOM	4769	CG2	ILE	15	22.911	48.638	40.813	1.00 31.65	CPS6
ATOM	4770	CG1	ILE	15	22.655	46.333	41.752	1.00 32.16	CPS6
ATOM	4771	CD1	ILE	15	24.156	46.184	42.013	1.00 33.75	CPS6
ATOM	4772	C	ILE	15	22.113	49.843	43.236	1.00 32.92	CPS6
ATOM	4773	O	ILE	15	23.062	50.627	43.265	1.00 32.09	CPS6
ATOM	4774	N	ALA	16	20.851	50.254	43.201	1.00 33.77	CPS6
ATOM	4775	CA	ALA	16	20.520	51.677	43.194	1.00 36.34	CPS6
ATOM	4776	CB	ALA	16	19.014	51.860	43.063	1.00 36.06	CPS6
ATOM	4777	C	ALA	16	21.030	52.356	44.467	1.00 38.13	CPS6
ATOM	4778	O	ALA	16	21.491	53.498	44.427	1.00 38.48	CPS6
ATOM	4779	N	SER	17	20.951	51.648	45.590	1.00 40.20	CPS6
ATOM	4780	CA	SER	17	21.415	52.175	46.871	1.00 43.01	CPS6
ATOM	4781	CB	SER	17	20.959	51.268	48.017	1.00 43.08	CPS6
ATOM	4782	OG	SER	17	19.549	51.302	48.157	1.00 45.35	CPS6
ATOM	4783	C	SER	17	22.934	52.320	46.919	1.00 44.34	CPS6
ATOM	4784	O	SER	17	23.456	53.311	47.432	1.00 44.28	CPS6
ATOM	4785	N	MET	18	23.644	51.323	46.402	1.00 45.43	CPS6
ATOM	4786	CA	MET	18	25.100	51.370	46.390	1.00 47.02	CPS6
ATOM	4787	CB	MET	18	25.678	50.035	45.917	1.00 48.11	CPS6

FIG. 1A-84

ATOM	4788	CG	MET	18	25.502	48.901	46.906	1.00 49.87	CPS6
ATOM	4789	SD	MET	18	26.307	47.401	46.338	1.00 54.02	CPS6
ATOM	4790	CE	MET	18	24.997	46.663	45.390	1.00 52.20	CPS6
ATOM	4791	C	MET	18	25.586	52.485	45.475	1.00 47.28	CPS6
ATOM	4792	O	MET	18	26.533	53.196	45.799	1.00 47.27	CPS6
ATOM	4793	N	ALA	19	24.923	52.636	44.334	1.00 47.28	CPS6
ATOM	4794	CA	ALA	19	25.284	53.658	43.361	1.00 48.35	CPS6
ATOM	4795	CB	ALA	19	24.558	53.397	42.049	1.00 47.94	CPS6
ATOM	4796	C	ALA	19	24.956	55.059	43.867	1.00 49.67	CPS6
ATOM	4797	O	ALA	19	25.644	56.031	43.539	1.00 48.84	CPS6
ATOM	4798	N	GLY	20	23.895	55.159	44.659	1.00 50.28	CPS6
ATOM	4799	CA	GLY	20	23.501	56.448	45.188	1.00 52.81	CPS6
ATOM	4800	C	GLY	20	24.379	56.884	46.342	1.00 53.84	CPS6
ATOM	4801	O	GLY	20	24.504	58.077	46.612	1.00 54.96	CPS6
ATOM	4802	N	ARG	21	24.996	55.919	47.017	1.00 54.88	CPS6
ATOM	4803	CA	ARG	21	25.853	56.215	48.157	1.00 56.13	CPS6
ATOM	4804	CB	ARG	21	25.694	55.134	49.228	1.00 57.83	CPS6
ATOM	4805	CG	ARG	21	24.308	55.086	49.857	1.00 60.18	CPS6
ATOM	4806	CD	ARG	21	24.275	54.226	51.123	1.00 62.40	CPS6
ATOM	4807	NE	ARG	21	24.085	52.797	50.866	1.00 64.82	CPS6
ATOM	4808	CZ	ARG	21	25.003	51.979	50.352	1.00 65.81	CPS6
ATOM	4809	NH1	ARG	21	26.207	52.434	50.024	1.00 66.03	CPS6
ATOM	4810	NH2	ARG	21	24.714	50.695	50.175	1.00 65.70	CPS6
ATOM	4811	C	ARG	21	27.327	56.359	47.802	1.00 56.17	CPS6
ATOM	4812	O	ARG	21	28.113	56.882	48.591	1.00 56.98	CPS6
ATOM	4813	N	GLN	22	27.710	55.896	46.619	1.00 55.40	CPS6
ATOM	4814	CA	GLN	22	29.104	55.992	46.207	1.00 54.24	CPS6
ATOM	4815	CB	GLN	22	29.637	54.619	45.795	1.00 55.16	CPS6
ATOM	4816	CG	GLN	22	29.456	53.533	46.836	1.00 57.52	CPS6
ATOM	4817	CD	GLN	22	30.179	52.251	46.467	1.00 58.37	CPS6
ATOM	4818	OE1	GLN	22	30.060	51.236	47.154	1.00 59.62	CPS6
ATOM	4819	NE2	GLN	22	30.940	52.294	45.378	1.00 59.05	CPS6
ATOM	4820	C	GLN	22	29.281	56.953	45.044	1.00 52.16	CPS6
ATOM	4821	O	GLN	22	28.312	57.363	44.402	1.00 51.84	CPS6
ATOM	4822	N	LYS	23	30.531	57.325	44.793	1.00 49.79	CPS6
ATOM	4823	CA	LYS	23	30.848	58.203	43.679	1.00 47.03	CPS6
ATOM	4824	CB	LYS	23	31.906	59.240	44.078	1.00 48.67	CPS6
ATOM	4825	CG	LYS	23	32.117	60.319	43.025	1.00 50.00	CPS6
ATOM	4826	CD	LYS	23	33.404	61.106	43.232	1.00 51.39	CPS6
ATOM	4827	CE	LYS	23	33.384	61.925	44.506	1.00 52.42	CPS6
ATOM	4828	NZ	LYS	23	34.570	62.835	44.558	1.00 53.74	CPS6
ATOM	4829	C	LYS	23	31.406	57.280	42.595	1.00 43.64	CPS6
ATOM	4830	O	LYS	23	32.259	56.433	42.866	1.00 43.39	CPS6
ATOM	4831	N	ARG	24	30.898	57.421	41.379	1.00 40.62	CPS6
ATOM	4832	CA	ARG	24	31.363	56.603	40.266	1.00 38.09	CPS6
ATOM	4833	CB	ARG	24	32.806	56.991	39.919	1.00 38.24	CPS6
ATOM	4834	CG	ARG	24	32.935	58.400	39.340	1.00 38.55	CPS6
ATOM	4835	CD	ARG	24	34.348	58.672	38.853	1.00 38.30	CPS6
ATOM	4836	NE	ARG	24	35.297	58.859	39.948	1.00 39.05	CPS6
ATOM	4837	CZ	ARG	24	35.511	60.019	40.561	1.00 39.71	CPS6
ATOM	4838	NH1	ARG	24	34.846	61.108	40.190	1.00 39.61	CPS6
ATOM	4839	NH2	ARG	24	36.396	60.092	41.543	1.00 39.47	CPS6
ATOM	4840	C	ARG	24	31.266	55.086	40.500	1.00 35.99	CPS6
ATOM	4841	O	ARG	24	32.202	54.339	40.206	1.00 34.55	CPS6
ATOM	4842	N	PHE	25	30.135	54.627	41.026	1.00 33.55	CPS6
ATOM	4843	CA	PHE	25	29.959	53.196	41.251	1.00 31.77	CPS6
ATOM	4844	CB	PHE	25	28.647	52.938	42.012	1.00 32.24	CPS6

FIG. 1A-85

ATOM	4845	CG	PHE	25	28.331	51.481	42.211	1.00 31.39	CPS6
ATOM	4846	CD1	PHE	25	27.306	50.879	41.495	1.00 33.76	CPS6
ATOM	4847	CD2	PHE	25	29.069	50.709	43.102	1.00 32.67	CPS6
ATOM	4848	CE1	PHE	25	27.021	49.524	41.663	1.00 32.84	CPS6
ATOM	4849	CE2	PHE	25	28.794	49.354	43.277	1.00 32.53	CPS6
ATOM	4850	CZ	PHE	25	27.764	48.763	42.553	1.00 32.75	CPS6
ATOM	4851	C	PHE	25	29.943	52.489	39.887	1.00 30.17	CPS6
ATOM	4852	O	PHE	25	30.573	51.446	39.706	1.00 28.44	CPS6
ATOM	4853	N	ALA	26	29.236	53.074	38.923	1.00 29.20	CPS6
ATOM	4854	CA	ALA	26	29.158	52.484	37.592	1.00 28.94	CPS6
ATOM	4855	CB	ALA	26	28.244	53.319	36.697	1.00 29.36	CPS6
ATOM	4856	C	ALA	26	30.540	52.376	36.961	1.00 28.91	CPS6
ATOM	4857	O	ALA	26	30.857	51.378	36.325	1.00 26.93	CPS6
ATOM	4858	N	GLU	27	31.358	53.411	37.144	1.00 28.69	CPS6
ATOM	4859	CA	GLU	27	32.701	53.434	36.576	1.00 29.76	CPS6
ATOM	4860	CB	GLU	27	33.317	54.829	36.730	1.00 30.26	CPS6
ATOM	4861	CG	GLU	27	32.737	55.916	35.822	1.00 32.04	CPS6
ATOM	4862	CD	GLU	27	31.325	56.344	36.195	1.00 33.96	CPS6
ATOM	4863	OE1	GLU	27	30.902	56.135	37.353	1.00 32.41	CPS6
ATOM	4864	OE2	GLU	27	30.638	56.914	35.318	1.00 37.48	CPS6
ATOM	4865	C	GLU	27	33.622	52.399	37.224	1.00 29.59	CPS6
ATOM	4866	O	GLU	27	34.661	52.040	36.673	1.00 29.53	CPS6
ATOM	4867	N	ARG	28	33.243	51.927	38.402	1.00 30.48	CPS6
ATOM	4868	CA	ARG	28	34.040	50.934	39.107	1.00 32.10	CPS6
ATOM	4869	CB	ARG	28	33.782	51.051	40.611	1.00 35.59	CPS6
ATOM	4870	CG	ARG	28	34.480	50.013	41.467	1.00 40.15	CPS6
ATOM	4871	CD	ARG	28	34.042	50.172	42.911	1.00 44.70	CPS6
ATOM	4872	NE	ARG	28	33.719	48.891	43.529	1.00 48.06	CPS6
ATOM	4873	CZ	ARG	28	33.004	48.764	44.642	1.00 50.43	CPS6
ATOM	4874	NH1	ARG	28	32.535	49.845	45.258	1.00 51.09	CPS6
ATOM	4875	NH2	ARG	28	32.755	47.558	45.139	1.00 51.52	CPS6
ATOM	4876	C	ARG	28	33.677	49.526	38.621	1.00 30.71	CPS6
ATOM	4877	O	ARG	28	34.546	48.659	38.464	1.00 32.13	CPS6
ATOM	4878	N	ILE	29	32.391	49.316	38.364	1.00 28.03	CPS6
ATOM	4879	CA	ILE	29	31.891	48.016	37.922	1.00 26.37	CPS6
ATOM	4880	CB	ILE	29	30.387	47.854	38.270	1.00 25.85	CPS6
ATOM	4881	CG2	ILE	29	29.886	46.496	37.802	1.00 25.90	CPS6
ATOM	4882	CG1	ILE	29	30.164	48.051	39.776	1.00 27.54	CPS6
ATOM	4883	CD1	ILE	29	30.962	47.113	40.667	1.00 27.66	CPS6
ATOM	4884	C	ILE	29	32.030	47.746	36.421	1.00 25.65	CPS6
ATOM	4885	O	ILE	29	32.327	46.617	36.017	1.00 24.93	CPS6
ATOM	4886	N	LEU	30	31.820	48.784	35.609	1.00 23.77	CPS6
ATOM	4887	CA	LEU	30	31.844	48.651	34.158	1.00 24.32	CPS6
ATOM	4888	CB	LEU	30	30.665	49.429	33.567	1.00 24.16	CPS6
ATOM	4889	CG	LEU	30	29.282	49.141	34.169	1.00 25.20	CPS6
ATOM	4890	CD1	LEU	30	28.251	50.068	33.540	1.00 24.33	CPS6
ATOM	4891	CD2	LEU	30	28.898	47.695	33.927	1.00 23.57	CPS6
ATOM	4892	C	LEU	30	33.121	49.071	33.433	1.00 24.24	CPS6
ATOM	4893	O	LEU	30	33.820	49.996	33.845	1.00 23.43	CPS6
ATOM	4894	N	THR	31	33.404	48.376	32.341	1.00 23.91	CPS6
ATOM	4895	CA	THR	31	34.573	48.676	31.523	1.00 25.21	CPS6
ATOM	4896	CB	THR	31	34.999	47.461	30.695	1.00 25.51	CPS6
ATOM	4897	OG1	THR	31	33.972	47.150	29.739	1.00 24.34	CPS6
ATOM	4898	CG2	THR	31	35.245	46.265	31.597	1.00 24.28	CPS6
ATOM	4899	C	THR	31	34.219	49.798	30.553	1.00 26.00	CPS6
ATOM	4900	O	THR	31	33.071	50.247	30.490	1.00 25.37	CPS6
ATOM	4901	N	ARG	32	35.202	50.240	29.782	1.00 27.55	CPS6

FIG. 1A-86

ATOM	4902	CA	ARG	32	34.976	51.310	28.818	1.00	29.54	CPS6
ATOM	4903	CB	ARG	32	36.290	51.626	28.091	1.00	32.98	CPS6
ATOM	4904	CG	ARG	32	36.198	52.721	27.040	1.00	38.34	CPS6
ATOM	4905	CD	ARG	32	37.595	53.116	26.557	1.00	42.64	CPS6
ATOM	4906	NE	ARG	32	38.282	53.987	27.513	1.00	45.62	CPS6
ATOM	4907	CZ	ARG	32	38.009	55.281	27.677	1.00	47.09	CPS6
ATOM	4908	NH1	ARG	32	37.065	55.865	26.946	1.00	48.54	CPS6
ATOM	4909	NH2	ARG	32	38.675	55.992	28.576	1.00	48.16	CPS6
ATOM	4910	C	ARG	32	33.879	50.928	27.815	1.00	28.32	CPS6
ATOM	4911	O	ARG	32	32.969	51.711	27.544	1.00	27.76	CPS6
ATOM	4912	N	SER	33	33.966	49.719	27.275	1.00	27.75	CPS6
ATOM	4913	CA	SER	33	32.988	49.238	26.303	1.00	28.81	CPS6
ATOM	4914	CB	SER	33	33.386	47.828	25.835	1.00	30.61	CPS6
ATOM	4915	OG	SER	33	32.421	47.266	24.963	1.00	33.62	CPS6
ATOM	4916	C	SER	33	31.586	49.211	26.926	1.00	28.93	CPS6
ATOM	4917	O	SER	33	30.599	49.614	26.302	1.00	28.74	CPS6
ATOM	4918	N	GLU	34	31.508	48.733	28.160	1.00	26.50	CPS6
ATOM	4919	CA	GLU	34	30.237	48.650	28.866	1.00	27.17	CPS6
ATOM	4920	CB	GLU	34	30.405	47.814	30.137	1.00	25.92	CPS6
ATOM	4921	CG	GLU	34	30.649	46.339	29.830	1.00	25.85	CPS6
ATOM	4922	CD	GLU	34	30.989	45.521	31.064	1.00	25.48	CPS6
ATOM	4923	OE1	GLU	34	30.771	44.290	31.035	1.00	24.91	CPS6
ATOM	4924	OE2	GLU	34	31.479	46.102	32.057	1.00	23.64	CPS6
ATOM	4925	C	GLU	34	29.688	50.029	29.193	1.00	27.92	CPS6
ATOM	4926	O	GLU	34	28.492	50.276	29.026	1.00	28.34	CPS6
ATOM	4927	N	LEU	35	30.556	50.929	29.648	1.00	27.84	CPS6
ATOM	4928	CA	LEU	35	30.137	52.286	29.977	1.00	30.69	CPS6
ATOM	4929	CB	LEU	35	31.310	53.081	30.557	1.00	30.33	CPS6
ATOM	4930	CG	LEU	35	31.719	52.712	31.981	1.00	30.63	CPS6
ATOM	4931	CD1	LEU	35	33.062	53.354	32.327	1.00	30.22	CPS6
ATOM	4932	CD2	LEU	35	30.631	53.170	32.943	1.00	30.10	CPS6
ATOM	4933	C	LEU	35	29.583	53.012	28.756	1.00	32.12	CPS6
ATOM	4934	O	LEU	35	28.669	53.826	28.880	1.00	32.67	CPS6
ATOM	4935	N	ASP	36	30.140	52.730	27.579	1.00	34.02	CPS6
ATOM	4936	CA	ASP	36	29.656	53.376	26.362	1.00	36.28	CPS6
ATOM	4937	CB	ASP	36	30.457	52.928	25.131	1.00	38.02	CPS6
ATOM	4938	CG	ASP	36	31.801	53.636	25.016	1.00	41.17	CPS6
ATOM	4939	OD1	ASP	36	31.924	54.767	25.538	1.00	42.30	CPS6
ATOM	4940	OD2	ASP	36	32.730	53.073	24.391	1.00	43.23	CPS6
ATOM	4941	C	ASP	36	28.177	53.071	26.152	1.00	37.04	CPS6
ATOM	4942	O	ASP	36	27.411	53.945	25.756	1.00	38.21	CPS6
ATOM	4943	N	GLN	37	27.772	51.836	26.427	1.00	36.14	CPS6
ATOM	4944	CA	GLN	37	26.376	51.449	26.261	1.00	37.10	CPS6
ATOM	4945	CB	GLN	37	26.253	49.928	26.271	1.00	39.04	CPS6
ATOM	4946	CG	GLN	37	27.296	49.234	25.424	1.00	43.60	CPS6
ATOM	4947	CD	GLN	37	27.084	47.741	25.357	1.00	47.47	CPS6
ATOM	4948	OE1	GLN	37	26.134	47.268	24.726	1.00	50.58	CPS6
ATOM	4949	NE2	GLN	37	27.960	46.983	26.016	1.00	47.62	CPS6
ATOM	4950	C	GLN	37	25.535	52.042	27.389	1.00	36.39	CPS6
ATOM	4951	O	GLN	37	24.466	52.607	27.159	1.00	36.41	CPS6
ATOM	4952	N	TYR	38	26.045	51.909	28.608	1.00	35.09	CPS6
ATOM	4953	CA	TYR	38	25.395	52.405	29.813	1.00	35.03	CPS6
ATOM	4954	CB	TYR	38	26.346	52.199	31.000	1.00	33.56	CPS6
ATOM	4955	CG	TYR	38	25.868	52.724	32.330	1.00	32.55	CPS6
ATOM	4956	CD1	TYR	38	26.296	53.958	32.810	1.00	32.33	CPS6
ATOM	4957	CE1	TYR	38	25.882	54.427	34.057	1.00	33.78	CPS6
ATOM	4958	CD2	TYR	38	25.008	51.969	33.127	1.00	31.82	CPS6

FIG. 1A-87

ATOM	4959	CE2	TYR	38	24.590	52.423	34.367	1.00	32.17	CPS6
ATOM	4960	CZ	TYR	38	25.029	53.652	34.829	1.00	33.51	CPS6
ATOM	4961	OH	TYR	38	24.611	54.099	36.060	1.00	34.37	CPS6
ATOM	4962	C	TYR	38	24.978	53.872	29.714	1.00	36.19	CPS6
ATOM	4963	O	TYR	38	23.825	54.213	29.974	1.00	35.32	CPS6
ATOM	4964	N	TYR	39	25.917	54.733	29.335	1.00	37.73	CPS6
ATOM	4965	CA	TYR	39	25.649	56.168	29.229	1.00	39.75	CPS6
ATOM	4966	CB	TYR	39	26.922	56.925	28.838	1.00	39.88	CPS6
ATOM	4967	CG	TYR	39	28.029	56.896	29.873	1.00	40.44	CPS6
ATOM	4968	CD1	TYR	39	27.742	56.963	31.239	1.00	39.77	CPS6
ATOM	4969	CE1	TYR	39	28.762	56.991	32.188	1.00	39.44	CPS6
ATOM	4970	CD2	TYR	39	29.370	56.855	29.481	1.00	40.21	CPS6
ATOM	4971	CE2	TYR	39	30.399	56.884	30.420	1.00	39.93	CPS6
ATOM	4972	CZ	TYR	39	30.089	56.954	31.773	1.00	40.43	CPS6
ATOM	4973	OH	TYR	39	31.109	57.010	32.702	1.00	40.54	CPS6
ATOM	4974	C	TYR	39	24.538	56.546	28.254	1.00	41.06	CPS6
ATOM	4975	O	TYR	39	23.957	57.627	28.357	1.00	42.29	CPS6
ATOM	4976	N	GLU	40	24.239	55.668	27.307	1.00	42.33	CPS6
ATOM	4977	CA	GLU	40	23.199	55.965	26.331	1.00	44.33	CPS6
ATOM	4978	CB	GLU	40	23.541	55.323	24.986	1.00	46.05	CPS6
ATOM	4979	CG	GLU	40	24.916	55.689	24.466	1.00	50.15	CPS6
ATOM	4980	CD	GLU	40	25.203	55.088	23.105	1.00	52.92	CPS6
ATOM	4981	OE1	GLU	40	25.040	53.857	22.948	1.00	55.32	CPS6
ATOM	4982	OE2	GLU	40	25.599	55.848	22.191	1.00	54.91	CPS6
ATOM	4983	C	GLU	40	21.827	55.488	26.780	1.00	44.19	CPS6
ATOM	4984	O	GLU	40	20.854	55.629	26.041	1.00	44.77	CPS6
ATOM	4985	N	LEU	41	21.743	54.941	27.991	1.00	42.63	CPS6
ATOM	4986	CA	LEU	41	20.474	54.427	28.499	1.00	42.23	CPS6
ATOM	4987	CB	LEU	41	20.696	53.114	29.259	1.00	41.12	CPS6
ATOM	4988	CG	LEU	41	21.294	51.934	28.486	1.00	40.93	CPS6
ATOM	4989	CD1	LEU	41	21.524	50.777	29.446	1.00	39.97	CPS6
ATOM	4990	CD2	LEU	41	20.362	51.514	27.360	1.00	40.04	CPS6
ATOM	4991	C	LEU	41	19.736	55.392	29.410	1.00	41.84	CPS6
ATOM	4992	O	LEU	41	20.317	56.335	29.934	1.00	41.86	CPS6
ATOM	4993	N	SER	42	18.447	55.129	29.597	1.00	42.32	CPS6
ATOM	4994	CA	SER	42	17.602	55.937	30.465	1.00	43.65	CPS6
ATOM	4995	CB	SER	42	16.134	55.578	30.252	1.00	43.85	CPS6
ATOM	4996	OG	SER	42	15.871	54.269	30.726	1.00	44.29	CPS6
ATOM	4997	C	SER	42	17.983	55.620	31.902	1.00	43.88	CPS6
ATOM	4998	O	SER	42	18.661	54.626	32.157	1.00	44.22	CPS6
ATOM	4999	N	GLU	43	17.540	56.447	32.843	1.00	43.94	CPS6
ATOM	5000	CA	GLU	43	17.860	56.216	34.248	1.00	44.69	CPS6
ATOM	5001	CB	GLU	43	17.195	57.266	35.147	1.00	47.52	CPS6
ATOM	5002	CG	GLU	43	17.466	57.033	36.632	1.00	51.04	CPS6
ATOM	5003	CD	GLU	43	16.733	58.002	37.546	1.00	53.92	CPS6
ATOM	5004	OE1	GLU	43	15.480	57.965	37.596	1.00	55.09	CPS6
ATOM	5005	OE2	GLU	43	17.418	58.802	38.221	1.00	55.13	CPS6
ATOM	5006	C	GLU	43	17.411	54.828	34.687	1.00	43.76	CPS6
ATOM	5007	O	GLU	43	18.123	54.143	35.419	1.00	43.62	CPS6
ATOM	5008	N	LYS	44	16.227	54.419	34.244	1.00	42.65	CPS6
ATOM	5009	CA	LYS	44	15.699	53.110	34.601	1.00	42.18	CPS6
ATOM	5010	CB	LYS	44	14.244	52.980	34.151	1.00	43.86	CPS6
ATOM	5011	CG	LYS	44	13.612	51.643	34.508	1.00	45.75	CPS6
ATOM	5012	CD	LYS	44	12.155	51.590	34.086	1.00	47.40	CPS6
ATOM	5013	CE	LYS	44	11.521	50.267	34.474	1.00	48.83	CPS6
ATOM	5014	NZ	LYS	44	10.076	50.213	34.107	1.00	50.91	CPS6
ATOM	5015	C	LYS	44	16.521	51.994	33.966	1.00	40.95	CPS6

FIG. 1A-88

ATOM	5016	O	LYS	44	16.952	51.064	34.645	1.00	40.09	CPS6
ATOM	5017	N	ARG	45	16.722	52.091	32.656	1.00	39.93	CPS6
ATOM	5018	CA	ARG	45	17.490	51.095	31.923	1.00	38.26	CPS6
ATOM	5019	CB	ARG	45	17.518	51.437	30.434	1.00	40.94	CPS6
ATOM	5020	CG	ARG	45	16.178	51.285	29.736	1.00	45.37	CPS6
ATOM	5021	CD	ARG	45	15.796	49.825	29.572	1.00	48.47	CPS6
ATOM	5022	NE	ARG	45	16.746	49.092	28.732	1.00	52.03	CPS6
ATOM	5023	CZ	ARG	45	17.047	49.411	27.475	1.00	54.07	CPS6
ATOM	5024	NH1	ARG	45	16.480	50.459	26.888	1.00	55.15	CPS6
ATOM	5025	NH2	ARG	45	17.917	48.672	26.796	1.00	55.63	CPS6
ATOM	5026	C	ARG	45	18.915	50.992	32.441	1.00	35.74	CPS6
ATOM	5027	O	ARG	45	19.524	49.926	32.374	1.00	33.44	CPS6
ATOM	5028	N	LYS	46	19.456	52.098	32.945	1.00	33.77	CPS6
ATOM	5029	CA	LYS	46	20.814	52.075	33.466	1.00	32.86	CPS6
ATOM	5030	CB	LYS	46	21.311	53.489	33.787	1.00	33.65	CPS6
ATOM	5031	CG	LYS	46	21.636	54.270	32.529	1.00	35.15	CPS6
ATOM	5032	CD	LYS	46	22.700	55.318	32.752	1.00	38.55	CPS6
ATOM	5033	CE	LYS	46	22.185	56.492	33.528	1.00	38.97	CPS6
ATOM	5034	NZ	LYS	46	22.923	57.716	33.075	1.00	40.88	CPS6
ATOM	5035	C	LYS	46	20.904	51.196	34.693	1.00	31.44	CPS6
ATOM	5036	O	LYS	46	21.841	50.415	34.832	1.00	30.69	CPS6
ATOM	5037	N	ASN	47	19.927	51.310	35.585	1.00	30.34	CPS6
ATOM	5038	CA	ASN	47	19.935	50.486	36.788	1.00	29.82	CPS6
ATOM	5039	CB	ASN	47	18.779	50.880	37.713	1.00	30.59	CPS6
ATOM	5040	CG	ASN	47	18.683	49.983	38.935	1.00	32.30	CPS6
ATOM	5041	OD1	ASN	47	19.510	50.057	39.851	1.00	33.45	CPS6
ATOM	5042	ND2	ASN	47	17.675	49.119	38.950	1.00	34.07	CPS6
ATOM	5043	C	ASN	47	19.821	49.003	36.401	1.00	28.64	CPS6
ATOM	5044	O	ASN	47	20.503	48.154	36.970	1.00	28.65	CPS6
ATOM	5045	N	GLU	48	18.972	48.700	35.424	1.00	28.08	CPS6
ATOM	5046	CA	GLU	48	18.796	47.319	34.969	1.00	28.15	CPS6
ATOM	5047	CB	GLU	48	17.680	47.234	33.927	1.00	31.68	CPS6
ATOM	5048	CG	GLU	48	16.301	47.618	34.448	1.00	36.94	CPS6
ATOM	5049	CD	GLU	48	15.246	47.631	33.352	1.00	40.49	CPS6
ATOM	5050	OE1	GLU	48	14.076	47.950	33.661	1.00	42.57	CPS6
ATOM	5051	OE2	GLU	48	15.585	47.325	32.185	1.00	40.94	CPS6
ATOM	5052	C	GLU	48	20.085	46.783	34.344	1.00	27.02	CPS6
ATOM	5053	O	GLU	48	20.489	45.646	34.598	1.00	25.06	CPS6
ATOM	5054	N	PHE	49	20.714	47.613	33.515	1.00	25.48	CPS6
ATOM	5055	CA	PHE	49	21.949	47.243	32.830	1.00	26.00	CPS6
ATOM	5056	CB	PHE	49	22.351	48.358	31.858	1.00	26.69	CPS6
ATOM	5057	CG	PHE	49	23.585	48.058	31.057	1.00	27.23	CPS6
ATOM	5058	CD1	PHE	49	23.497	47.397	29.838	1.00	28.29	CPS6
ATOM	5059	CD2	PHE	49	24.835	48.455	31.515	1.00	26.82	CPS6
ATOM	5060	CE1	PHE	49	24.640	47.142	29.081	1.00	28.93	CPS6
ATOM	5061	CE2	PHE	49	25.987	48.202	30.765	1.00	27.94	CPS6
ATOM	5062	CZ	PHE	49	25.886	47.548	29.550	1.00	28.38	CPS6
ATOM	5063	C	PHE	49	23.066	46.997	33.837	1.00	24.84	CPS6
ATOM	5064	O	PHE	49	23.739	45.966	33.789	1.00	25.50	CPS6
ATOM	5065	N	LEU	50	23.264	47.946	34.747	1.00	24.16	CPS6
ATOM	5066	CA	LEU	50	24.296	47.824	35.773	1.00	22.97	CPS6
ATOM	5067	CB	LEU	50	24.304	49.088	36.647	1.00	24.37	CPS6
ATOM	5068	CG	LEU	50	25.348	49.178	37.759	1.00	25.79	CPS6
ATOM	5069	CD1	LEU	50	26.760	49.145	37.149	1.00	26.03	CPS6
ATOM	5070	CD2	LEU	50	25.141	50.471	38.537	1.00	26.29	CPS6
ATOM	5071	C	LEU	50	24.081	46.583	36.653	1.00	21.87	CPS6
ATOM	5072	O	LEU	50	25.022	45.839	36.939	1.00	21.43	CPS6

FIG. 1A-89

ATOM	5073	N	ALA	51	22.844	46.364	37.089	1.00	21.05	CPS6
ATOM	5074	CA	ALA	51	22.524	45.218	37.940	1.00	21.01	CPS6
ATOM	5075	CB	ALA	51	21.038	45.271	38.346	1.00	20.12	CPS6
ATOM	5076	C	ALA	51	22.829	43.894	37.223	1.00	20.25	CPS6
ATOM	5077	O	ALA	51	23.351	42.955	37.825	1.00	20.85	CPS6
ATOM	5078	N	GLY	52	22.493	43.830	35.943	1.00	21.02	CPS6
ATOM	5079	CA	GLY	52	22.742	42.624	35.164	1.00	20.99	CPS6
ATOM	5080	C	GLY	52	24.232	42.376	34.989	1.00	22.24	CPS6
ATOM	5081	O	GLY	52	24.688	41.232	35.044	1.00	21.77	CPS6
ATOM	5082	N	ARG	53	24.992	43.444	34.764	1.00	22.45	CPS6
ATOM	5083	CA	ARG	53	26.442	43.317	34.600	1.00	22.02	CPS6
ATOM	5084	CB	ARG	53	27.051	44.624	34.093	1.00	23.58	CPS6
ATOM	5085	CG	ARG	53	26.831	44.875	32.628	1.00	26.56	CPS6
ATOM	5086	CD	ARG	53	27.406	43.749	31.834	1.00	28.57	CPS6
ATOM	5087	NE	ARG	53	27.764	44.164	30.483	1.00	32.59	CPS6
ATOM	5088	CZ	ARG	53	26.903	44.301	29.481	1.00	32.51	CPS6
ATOM	5089	NH1	ARG	53	25.606	44.053	29.676	1.00	29.51	CPS6
ATOM	5090	NH2	ARG	53	27.352	44.666	28.277	1.00	29.31	CPS6
ATOM	5091	C	ARG	53	27.081	42.951	35.926	1.00	22.03	CPS6
ATOM	5092	O	ARG	53	28.014	42.159	35.983	1.00	22.12	CPS6
ATOM	5093	N	PHE	54	26.576	43.541	37.000	1.00	20.72	CPS6
ATOM	5094	CA	PHE	54	27.089	43.253	38.322	1.00	21.84	CPS6
ATOM	5095	CB	PHE	54	26.391	44.144	39.347	1.00	23.57	CPS6
ATOM	5096	CG	PHE	54	26.843	43.925	40.756	1.00	24.76	CPS6
ATOM	5097	CD1	PHE	54	26.202	42.996	41.571	1.00	26.78	CPS6
ATOM	5098	CD2	PHE	54	27.896	44.666	41.282	1.00	26.87	CPS6
ATOM	5099	CE1	PHE	54	26.603	42.815	42.886	1.00	27.91	CPS6
ATOM	5100	CE2	PHE	54	28.302	44.491	42.592	1.00	26.99	CPS6
ATOM	5101	CZ	PHE	54	27.656	43.567	43.397	1.00	27.41	CPS6
ATOM	5102	C	PHE	54	26.865	41.777	38.647	1.00	21.21	CPS6
ATOM	5103	O	PHE	54	27.768	41.097	39.123	1.00	20.78	CPS6
ATOM	5104	N	ALA	55	25.665	41.277	38.381	1.00	20.89	CPS6
ATOM	5105	CA	ALA	55	25.374	39.872	38.669	1.00	20.22	CPS6
ATOM	5106	CB	ALA	55	23.892	39.574	38.441	1.00	19.35	CPS6
ATOM	5107	C	ALA	55	26.224	38.955	37.805	1.00	18.66	CPS6
ATOM	5108	O	ALA	55	26.716	37.923	38.278	1.00	19.74	CPS6
ATOM	5109	N	ALA	56	26.395	39.314	36.538	1.00	18.06	CPS6
ATOM	5110	CA	ALA	56	27.195	38.488	35.639	1.00	18.21	CPS6
ATOM	5111	CB	ALA	56	27.134	39.041	34.198	1.00	18.23	CPS6
ATOM	5112	C	ALA	56	28.648	38.387	36.101	1.00	18.83	CPS6
ATOM	5113	O	ALA	56	29.259	37.307	36.057	1.00	17.66	CPS6
ATOM	5114	N	LYS	57	29.207	39.508	36.549	1.00	19.03	CPS6
ATOM	5115	CA	LYS	57	30.592	39.513	37.012	1.00	18.37	CPS6
ATOM	5116	CB	LYS	57	31.101	40.958	37.085	1.00	19.18	CPS6
ATOM	5117	CG	LYS	57	31.179	41.574	35.689	1.00	19.49	CPS6
ATOM	5118	CD	LYS	57	31.775	42.975	35.676	1.00	23.00	CPS6
ATOM	5119	CE	LYS	57	31.663	43.579	34.285	1.00	20.60	CPS6
ATOM	5120	NZ	LYS	57	32.580	44.729	34.103	1.00	21.27	CPS6
ATOM	5121	C	LYS	57	30.745	38.785	38.344	1.00	19.47	CPS6
ATOM	5122	O	LYS	57	31.739	38.084	38.557	1.00	20.88	CPS6
ATOM	5123	N	GLU	58	29.773	38.942	39.245	1.00	19.43	CPS6
ATOM	5124	CA	GLU	58	29.821	38.212	40.512	1.00	21.77	CPS6
ATOM	5125	CB	GLU	58	28.640	38.591	41.419	1.00	22.85	CPS6
ATOM	5126	CG	GLU	58	28.746	39.965	42.066	1.00	27.74	CPS6
ATOM	5127	CD	GLU	58	29.884	40.060	43.079	1.00	30.88	CPS6
ATOM	5128	OE1	GLU	58	30.148	41.173	43.580	1.00	34.74	CPS6
ATOM	5129	OE2	GLU	58	30.517	39.028	43.378	1.00	34.50	CPS6

FIG. 1A-90

ATOM	5130	C	GLU	58	29.745	36.711	40.199	1.00 21.81	CPS6
ATOM	5131	O	GLU	58	30.494	35.900	40.767	1.00 21.58	CPS6
ATOM	5132	N	ALA	59	28.833	36.332	39.305	1.00 20.31	CPS6
ATOM	5133	CA	ALA	59	28.704	34.917	38.958	1.00 20.01	CPS6
ATOM	5134	CB	ALA	59	27.557	34.709	37.956	1.00 19.39	CPS6
ATOM	5135	C	ALA	59	30.015	34.398	38.370	1.00 20.62	CPS6
ATOM	5136	O	ALA	59	30.463	33.289	38.693	1.00 21.08	CPS6
ATOM	5137	N	PHE	60	30.625	35.192	37.497	1.00 18.52	CPS6
ATOM	5138	CA	PHE	60	31.886	34.784	36.891	1.00 20.21	CPS6
ATOM	5139	CB	PHE	60	32.359	35.819	35.863	1.00 19.79	CPS6
ATOM	5140	CG	PHE	60	33.690	35.482	35.248	1.00 21.99	CPS6
ATOM	5141	CD1	PHE	60	33.768	34.653	34.133	1.00 19.74	CPS6
ATOM	5142	CD2	PHE	60	34.874	35.925	35.842	1.00 22.16	CPS6
ATOM	5143	CE1	PHE	60	35.010	34.264	33.618	1.00 23.98	CPS6
ATOM	5144	CE2	PHE	60	36.117	35.542	35.339	1.00 23.86	CPS6
ATOM	5145	CZ	PHE	60	36.187	34.709	34.227	1.00 23.24	CPS6
ATOM	5146	C	PHE	60	32.970	34.614	37.961	1.00 21.37	CPS6
ATOM	5147	O	PHE	60	33.724	33.638	37.938	1.00 22.00	CPS6
ATOM	5148	N	SER	61	33.048	35.565	38.891	1.00 21.71	CPS6
ATOM	5149	CA	SER	61	34.065	35.516	39.945	1.00 23.80	CPS6
ATOM	5150	CB	SER	61	34.003	36.772	40.824	1.00 23.70	CPS6
ATOM	5151	OG	SER	61	32.938	36.694	41.753	1.00 25.60	CPS6
ATOM	5152	C	SER	61	33.912	34.284	40.824	1.00 24.14	CPS6
ATOM	5153	O	SER	61	34.897	33.786	41.386	1.00 25.44	CPS6
ATOM	5154	N	LYS	62	32.683	33.800	40.957	1.00 23.98	CPS6
ATOM	5155	CA	LYS	62	32.425	32.609	41.764	1.00 25.63	CPS6
ATOM	5156	CB	LYS	62	30.946	32.566	42.174	1.00 25.79	CPS6
ATOM	5157	CG	LYS	62	30.601	33.735	43.097	1.00 29.14	CPS6
ATOM	5158	CD	LYS	62	29.112	33.966	43.281	1.00 32.29	CPS6
ATOM	5159	CE	LYS	62	28.492	32.995	44.255	1.00 34.95	CPS6
ATOM	5160	NZ	LYS	62	27.224	33.584	44.793	1.00 38.32	CPS6
ATOM	5161	C	LYS	62	32.830	31.358	40.995	1.00 26.22	CPS6
ATOM	5162	O	LYS	62	33.397	30.424	41.568	1.00 25.89	CPS6
ATOM	5163	N	ALA	63	32.556	31.343	39.693	1.00 24.67	CPS6
ATOM	5164	CA	ALA	63	32.936	30.209	38.861	1.00 24.83	CPS6
ATOM	5165	CB	ALA	63	32.345	30.359	37.464	1.00 24.34	CPS6
ATOM	5166	C	ALA	63	34.459	30.174	38.780	1.00 26.66	CPS6
ATOM	5167	O	ALA	63	35.064	29.105	38.737	1.00 26.11	CPS6
ATOM	5168	N	PHE	64	35.071	31.354	38.762	1.00 26.12	CPS6
ATOM	5169	CA	PHE	64	36.526	31.467	38.692	1.00 28.50	CPS6
ATOM	5170	CB	PHE	64	36.919	32.925	38.445	1.00 28.06	CPS6
ATOM	5171	CG	PHE	64	38.341	33.104	37.992	1.00 29.52	CPS6
ATOM	5172	CD1	PHE	64	38.760	32.606	36.765	1.00 29.61	CPS6
ATOM	5173	CD2	PHE	64	39.251	33.787	38.787	1.00 29.01	CPS6
ATOM	5174	CE1	PHE	64	40.072	32.787	36.329	1.00 32.11	CPS6
ATOM	5175	CE2	PHE	64	40.565	33.973	38.362	1.00 30.85	CPS6
ATOM	5176	CZ	PHE	64	40.975	33.473	37.130	1.00 31.27	CPS6
ATOM	5177	C	PHE	64	37.176	30.953	39.981	1.00 29.90	CPS6
ATOM	5178	O	PHE	64	38.376	30.661	40.003	1.00 30.91	CPS6
ATOM	5179	N	GLY	65	36.377	30.858	41.043	1.00 31.52	CPS6
ATOM	5180	CA	GLY	65	36.845	30.349	42.322	1.00 34.23	CPS6
ATOM	5181	C	GLY	65	37.435	31.337	43.315	1.00 36.45	CPS6
ATOM	5182	O	GLY	65	37.726	30.968	44.456	1.00 37.62	CPS6
ATOM	5183	N	THR	66	37.593	32.592	42.902	1.00 36.65	CPS6
ATOM	5184	CA	THR	66	38.195	33.616	43.755	1.00 36.52	CPS6
ATOM	5185	CB	THR	66	39.272	34.385	42.978	1.00 36.52	CPS6
ATOM	5186	OG1	THR	66	38.648	35.112	41.908	1.00 36.34	CPS6

FIG. 1A-91


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ATOM   5187  CG2 THR    66      40.297  33.429  42.389  1.00 36.79      CPS6
ATOM   5188  C   THR    66      37.243  34.666  44.329  1.00 36.19      CPS6
ATOM   5189  O   THR    66      37.475  35.193  45.419  1.00 35.77      CPS6
ATOM   5190  N   GLY    67      36.175  34.973  43.599  1.00 35.09      CPS6
ATOM   5191  CA  GLY    67      35.266  36.011  44.046  1.00 33.07      CPS6
ATOM   5192  C   GLY    67      35.944  37.308  43.634  1.00 32.90      CPS6
ATOM   5193  O   GLY    67      37.083  37.269  43.168  1.00 32.07      CPS6
ATOM   5194  N   ILE    68      35.264  38.446  43.766  1.00 32.48      CPS6
ATOM   5195  CA  ILE    68      35.878  39.721  43.397  1.00 32.14      CPS6
ATOM   5196  CB  ILE    68      34.821  40.823  43.170  1.00 31.75      CPS6
ATOM   5197  CG2 ILE    68      35.509  42.167  42.928  1.00 32.21      CPS6
ATOM   5198  CG1 ILE    68      33.941  40.463  41.967  1.00 30.11      CPS6
ATOM   5199  CD1 ILE    68      34.697  40.354  40.642  1.00 30.32      CPS6
ATOM   5200  C   ILE    68      36.796  40.150  44.536  1.00 33.67      CPS6
ATOM   5201  O   ILE    68      36.370  40.206  45.692  1.00 33.24      CPS6
ATOM   5202  N   GLY    69      38.050  40.443  44.207  1.00 34.42      CPS6
ATOM   5203  CA  GLY    69      39.002  40.845  45.226  1.00 37.25      CPS6
ATOM   5204  C   GLY    69      40.431  40.946  44.719  1.00 38.28      CPS6
ATOM   5205  O   GLY    69      40.669  41.302  43.567  1.00 38.30      CPS6
ATOM   5206  N   ALA    70      41.386  40.609  45.579  1.00 38.96      CPS6
ATOM   5207  CA  ALA    70      42.800  40.684  45.233  1.00 39.69      CPS6
ATOM   5208  CB  ALA    70      43.644  40.198  46.415  1.00 40.64      CPS6
ATOM   5209  C   ALA    70      43.208  39.939  43.965  1.00 39.83      CPS6
ATOM   5210  O   ALA    70      44.175  40.322  43.311  1.00 40.54      CPS6
ATOM   5211  N   GLN    71      42.481  38.885  43.605  1.00 39.94      CPS6
ATOM   5212  CA  GLN    71      42.834  38.115  42.411  1.00 39.34      CPS6
ATOM   5213  CB  GLN    71      42.773  36.614  42.709  1.00 41.56      CPS6
ATOM   5214  CG  GLN    71      43.429  36.181  44.006  1.00 43.98      CPS6
ATOM   5215  CD  GLN    71      43.299  34.684  44.233  1.00 45.96      CPS6
ATOM   5216  OE1 GLN    71      43.901  33.880  43.515  1.00 48.14      CPS6
ATOM   5217  NE2 GLN    71      42.502  34.302  45.224  1.00 46.92      CPS6
ATOM   5218  C   GLN    71      41.972  38.381  41.176  1.00 37.54      CPS6
ATOM   5219  O   GLN    71      42.286  37.886  40.096  1.00 37.40      CPS6
ATOM   5220  N   LEU    72      40.898  39.154  41.326  1.00 35.40      CPS6
ATOM   5221  CA  LEU    72      39.998  39.428  40.204  1.00 33.24      CPS6
ATOM   5222  CB  LEU    72      39.029  38.257  40.026  1.00 31.49      CPS6
ATOM   5223  CG  LEU    72      38.647  37.600  38.692  1.00 32.42      CPS6
ATOM   5224  CD1 LEU    72      37.168  37.243  38.788  1.00 28.80      CPS6
ATOM   5225  CD2 LEU    72      38.919  38.478  37.487  1.00 30.34      CPS6
ATOM   5226  C   LEU    72      39.174  40.680  40.483  1.00 31.78      CPS6
ATOM   5227  O   LEU    72      38.496  40.758  41.502  1.00 32.54      CPS6
ATOM   5228  N   SER    73      39.217  41.652  39.583  1.00 30.85      CPS6
ATOM   5229  CA  SER    73      38.428  42.866  39.784  1.00 29.39      CPS6
ATOM   5230  CB  SER    73      39.289  44.113  39.615  1.00 30.61      CPS6
ATOM   5231  OG  SER    73      39.523  44.366  38.246  1.00 30.25      CPS6
ATOM   5232  C   SER    73      37.309  42.898  38.752  1.00 27.96      CPS6
ATOM   5233  O   SER    73      37.333  42.147  37.775  1.00 27.49      CPS6
ATOM   5234  N   PHE    74      36.322  43.760  38.975  1.00 26.79      CPS6
ATOM   5235  CA  PHE    74      35.213  43.888  38.034  1.00 26.21      CPS6
ATOM   5236  CB  PHE    74      34.219  44.938  38.534  1.00 25.48      CPS6
ATOM   5237  CG  PHE    74      33.366  44.472  39.676  1.00 26.75      CPS6
ATOM   5238  CD1 PHE    74      32.329  43.568  39.460  1.00 27.07      CPS6
ATOM   5239  CD2 PHE    74      33.582  44.949  40.967  1.00 27.57      CPS6
ATOM   5240  CE1 PHE    74      31.511  43.148  40.515  1.00 27.84      CPS6
ATOM   5241  CE2 PHE    74      32.770  44.534  42.030  1.00 28.92      CPS6
ATOM   5242  CZ  PHE    74      31.732  43.634  41.801  1.00 27.85      CPS6
ATOM   5243  C   PHE    74      35.731  44.301  36.659  1.00 26.17      CPS6
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FIG. 1A-92

ATOM	5244	O	PHE	74	35.186	43.903	35.638	1.00	25.99	CPS6
ATOM	5245	N	GLN	75	36.793	45.103	36.638	1.00	25.96	CPS6
ATOM	5246	CA	GLN	75	37.365	45.583	35.384	1.00	27.32	CPS6
ATOM	5247	CB	GLN	75	38.374	46.703	35.665	1.00	27.52	CPS6
ATOM	5248	CG	GLN	75	37.754	47.960	36.271	1.00	30.15	CPS6
ATOM	5249	CD	GLN	75	36.770	48.648	35.339	1.00	30.80	CPS6
ATOM	5250	OE1	GLN	75	37.052	48.857	34.159	1.00	31.37	CPS6
ATOM	5251	NE2	GLN	75	35.618	49.019	35.871	1.00	34.02	CPS6
ATOM	5252	C	GLN	75	38.024	44.498	34.530	1.00	26.97	CPS6
ATOM	5253	O	GLN	75	38.199	44.679	33.329	1.00	26.86	CPS6
ATOM	5254	N	ASP	76	38.382	43.377	35.150	1.00	27.98	CPS6
ATOM	5255	CA	ASP	76	39.004	42.258	34.437	1.00	27.78	CPS6
ATOM	5256	CB	ASP	76	39.644	41.271	35.421	1.00	29.90	CPS6
ATOM	5257	CG	ASP	76	40.883	41.813	36.091	1.00	31.18	CPS6
ATOM	5258	OD1	ASP	76	41.690	42.457	35.397	1.00	35.07	CPS6
ATOM	5259	OD2	ASP	76	41.059	41.570	37.307	1.00	32.81	CPS6
ATOM	5260	C	ASP	76	37.969	41.474	33.633	1.00	27.27	CPS6
ATOM	5261	O	ASP	76	38.314	40.671	32.764	1.00	26.16	CPS6
ATOM	5262	N	ILE	77	36.696	41.705	33.930	1.00	26.25	CPS6
ATOM	5263	CA	ILE	77	35.616	40.966	33.272	1.00	25.67	CPS6
ATOM	5264	CB	ILE	77	34.682	40.360	34.335	1.00	25.40	CPS6
ATOM	5265	CG2	ILE	77	33.688	39.404	33.681	1.00	24.95	CPS6
ATOM	5266	CG1	ILE	77	35.511	39.639	35.400	1.00	23.36	CPS6
ATOM	5267	CD1	ILE	77	34.798	39.549	36.758	1.00	23.84	CPS6
ATOM	5268	C	ILE	77	34.785	41.871	32.372	1.00	25.23	CPS6
ATOM	5269	O	ILE	77	34.326	42.916	32.809	1.00	26.66	CPS6
ATOM	5270	N	GLU	78	34.579	41.473	31.123	1.00	24.36	CPS6
ATOM	5271	CA	GLU	78	33.794	42.296	30.217	1.00	23.95	CPS6
ATOM	5272	CB	GLU	78	34.689	42.928	29.151	1.00	23.23	CPS6
ATOM	5273	CG	GLU	78	33.936	43.867	28.231	1.00	25.47	CPS6
ATOM	5274	CD	GLU	78	34.858	44.740	27.406	1.00	28.41	CPS6
ATOM	5275	OE1	GLU	78	35.313	44.287	26.331	1.00	28.29	CPS6
ATOM	5276	OE2	GLU	78	35.133	45.880	27.844	1.00	29.93	CPS6
ATOM	5277	C	GLU	78	32.698	41.501	29.523	1.00	23.31	CPS6
ATOM	5278	O	GLU	78	32.951	40.411	29.013	1.00	23.66	CPS6
ATOM	5279	N	ILE	79	31.481	42.045	29.519	1.00	23.40	CPS6
ATOM	5280	CA	ILE	79	30.376	41.377	28.843	1.00	22.82	CPS6
ATOM	5281	CB	ILE	79	29.074	41.348	29.696	1.00	22.78	CPS6
ATOM	5282	CG2	ILE	79	27.899	40.913	28.834	1.00	23.83	CPS6
ATOM	5283	CG1	ILE	79	29.214	40.370	30.871	1.00	23.62	CPS6
ATOM	5284	CD1	ILE	79	29.978	40.908	32.041	1.00	26.29	CPS6
ATOM	5285	C	ILE	79	30.081	42.125	27.551	1.00	22.89	CPS6
ATOM	5286	O	ILE	79	29.992	43.352	27.547	1.00	21.79	CPS6
ATOM	5287	N	ARG	80	29.969	41.383	26.456	1.00	22.11	CPS6
ATOM	5288	CA	ARG	80	29.625	41.957	25.152	1.00	24.89	CPS6
ATOM	5289	CB	ARG	80	30.781	41.821	24.147	1.00	28.30	CPS6
ATOM	5290	CG	ARG	80	32.171	41.662	24.758	1.00	34.49	CPS6
ATOM	5291	CD	ARG	80	33.065	42.894	24.630	1.00	37.92	CPS6
ATOM	5292	NE	ARG	80	33.175	43.397	23.267	1.00	39.97	CPS6
ATOM	5293	CZ	ARG	80	34.078	44.291	22.857	1.00	39.55	CPS6
ATOM	5294	NH1	ARG	80	34.981	44.787	23.697	1.00	38.56	CPS6
ATOM	5295	NH2	ARG	80	34.050	44.724	21.604	1.00	37.96	CPS6
ATOM	5296	C	ARG	80	28.445	41.119	24.657	1.00	24.70	CPS6
ATOM	5297	O	ARG	80	28.130	40.095	25.249	1.00	22.24	CPS6
ATOM	5298	N	LYS	81	27.776	41.551	23.592	1.00	26.22	CPS6
ATOM	5299	CA	LYS	81	26.664	40.770	23.055	1.00	28.06	CPS6
ATOM	5300	CB	LYS	81	25.346	41.547	23.140	1.00	30.47	CPS6

FIG. 1A-93

ATOM	5301	CG	LYS	81	24.745	41.614	24.542	1.00	34.14	CPS6
ATOM	5302	CD	LYS	81	23.460	42.439	24.545	1.00	37.71	CPS6
ATOM	5303	CE	LYS	81	22.985	42.787	25.963	1.00	39.78	CPS6
ATOM	5304	NZ	LYS	81	22.435	41.636	26.736	1.00	39.75	CPS6
ATOM	5305	C	LYS	81	26.962	40.409	21.608	1.00	29.13	CPS6
ATOM	5306	O	LYS	81	27.536	41.222	20.876	1.00	29.46	CPS6
ATOM	5307	N	ASP	82	26.602	39.193	21.197	1.00	29.17	CPS6
ATOM	5308	CA	ASP	82	26.861	38.783	19.824	1.00	31.09	CPS6
ATOM	5309	CB	ASP	82	27.044	37.255	19.707	1.00	29.73	CPS6
ATOM	5310	CG	ASP	82	25.751	36.464	19.877	1.00	28.91	CPS6
ATOM	5311	OD1	ASP	82	24.646	37.045	19.861	1.00	26.18	CPS6
ATOM	5312	OD2	ASP	82	25.861	35.226	20.012	1.00	28.29	CPS6
ATOM	5313	C	ASP	82	25.775	39.283	18.891	1.00	31.70	CPS6
ATOM	5314	O	ASP	82	24.909	40.051	19.306	1.00	32.19	CPS6
ATOM	5315	N	GLN	83	25.821	38.852	17.634	1.00	35.43	CPS6
ATOM	5316	CA	GLN	83	24.854	39.300	16.634	1.00	37.80	CPS6
ATOM	5317	CB	GLN	83	25.222	38.738	15.252	1.00	40.89	CPS6
ATOM	5318	CG	GLN	83	25.267	37.219	15.164	1.00	44.70	CPS6
ATOM	5319	CD	GLN	83	26.534	36.612	15.755	1.00	47.79	CPS6
ATOM	5320	OE1	GLN	83	26.642	35.388	15.889	1.00	49.81	CPS6
ATOM	5321	NE2	GLN	83	27.503	37.461	16.101	1.00	48.69	CPS6
ATOM	5322	C	GLN	83	23.400	38.966	16.965	1.00	38.04	CPS6
ATOM	5323	O	GLN	83	22.481	39.641	16.499	1.00	38.72	CPS6
ATOM	5324	N	ASN	84	23.182	37.933	17.772	1.00	36.73	CPS6
ATOM	5325	CA	ASN	84	21.822	37.564	18.146	1.00	35.24	CPS6
ATOM	5326	CB	ASN	84	21.701	36.049	18.292	1.00	35.98	CPS6
ATOM	5327	CG	ASN	84	21.864	35.331	16.979	1.00	37.29	CPS6
ATOM	5328	OD1	ASN	84	21.242	35.699	15.977	1.00	39.43	CPS6
ATOM	5329	ND2	ASN	84	22.694	34.298	16.968	1.00	36.91	CPS6
ATOM	5330	C	ASN	84	21.400	38.234	19.447	1.00	33.77	CPS6
ATOM	5331	O	ASN	84	20.262	38.088	19.882	1.00	34.74	CPS6
ATOM	5332	N	GLY	85	22.322	38.963	20.067	1.00	31.96	CPS6
ATOM	5333	CA	GLY	85	22.011	39.635	21.315	1.00	30.32	CPS6
ATOM	5334	C	GLY	85	22.360	38.777	22.520	1.00	28.59	CPS6
ATOM	5335	O	GLY	85	22.022	39.112	23.655	1.00	28.08	CPS6
ATOM	5336	N	LYS	86	23.041	37.664	22.265	1.00	26.87	CPS6
ATOM	5337	CA	LYS	86	23.451	36.743	23.323	1.00	24.77	CPS6
ATOM	5338	CB	LYS	86	23.760	35.365	22.719	1.00	24.34	CPS6
ATOM	5339	CG	LYS	86	24.446	34.376	23.663	1.00	23.41	CPS6
ATOM	5340	CD	LYS	86	23.518	33.886	24.783	1.00	22.54	CPS6
ATOM	5341	CE	LYS	86	24.296	33.008	25.778	1.00	21.86	CPS6
ATOM	5342	NZ	LYS	86	23.395	32.379	26.784	1.00	21.67	CPS6
ATOM	5343	C	LYS	86	24.690	37.282	24.028	1.00	23.40	CPS6
ATOM	5344	O	LYS	86	25.709	37.558	23.390	1.00	22.20	CPS6
ATOM	5345	N	PRO	87	24.628	37.443	25.359	1.00	22.90	CPS6
ATOM	5346	CD	PRO	87	23.483	37.328	26.283	1.00	23.21	CPS6
ATOM	5347	CA	PRO	87	25.820	37.956	26.050	1.00	21.73	CPS6
ATOM	5348	CB	PRO	87	25.281	38.351	27.427	1.00	23.57	CPS6
ATOM	5349	CG	PRO	87	24.166	37.350	27.648	1.00	23.73	CPS6
ATOM	5350	C	PRO	87	26.945	36.924	26.167	1.00	21.97	CPS6
ATOM	5351	O	PRO	87	26.693	35.724	26.260	1.00	19.28	CPS6
ATOM	5352	N	TYR	88	28.192	37.393	26.124	1.00	21.22	CPS6
ATOM	5353	CA	TYR	88	29.333	36.504	26.308	1.00	20.65	CPS6
ATOM	5354	CB	TYR	88	29.881	35.972	24.980	1.00	22.01	CPS6
ATOM	5355	CG	TYR	88	30.434	37.009	24.036	1.00	21.99	CPS6
ATOM	5356	CD1	TYR	88	31.796	37.317	24.021	1.00	25.46	CPS6
ATOM	5357	CE1	TYR	88	32.310	38.251	23.121	1.00	24.59	CPS6

FIG. 1A-94

ATOM	5358	CD2	TYR	88	29.600	37.666	23.132	1.00	25.11	CPS6
ATOM	5359	CE2	TYR	88	30.105	38.601	22.234	1.00	25.50	CPS6
ATOM	5360	CZ	TYR	88	31.459	38.887	22.235	1.00	26.13	CPS6
ATOM	5361	OH	TYR	88	31.947	39.824	21.351	1.00	28.03	CPS6
ATOM	5362	C	TYR	88	30.382	37.287	27.062	1.00	21.33	CPS6
ATOM	5363	O	TYR	88	30.415	38.512	27.009	1.00	22.02	CPS6
ATOM	5364	N	ILE	89	31.238	36.571	27.769	1.00	22.15	CPS6
ATOM	5365	CA	ILE	89	32.263	37.187	28.581	1.00	22.97	CPS6
ATOM	5366	CB	ILE	89	32.244	36.555	30.001	1.00	22.83	CPS6
ATOM	5367	CG2	ILE	89	33.564	36.820	30.736	1.00	22.49	CPS6
ATOM	5368	CG1	ILE	89	31.036	37.080	30.779	1.00	23.07	CPS6
ATOM	5369	CD1	ILE	89	30.876	36.460	32.168	1.00	23.21	CPS6
ATOM	5370	C	ILE	89	33.670	37.026	28.027	1.00	24.96	CPS6
ATOM	5371	O	ILE	89	33.990	35.997	27.435	1.00	24.10	CPS6
ATOM	5372	N	ILE	90	34.489	38.064	28.193	1.00	24.59	CPS6
ATOM	5373	CA	ILE	90	35.898	37.956	27.833	1.00	25.62	CPS6
ATOM	5374	CB	ILE	90	36.305	38.796	26.589	1.00	26.38	CPS6
ATOM	5375	CG2	ILE	90	35.630	38.229	25.360	1.00	26.74	CPS6
ATOM	5376	CG1	ILE	90	35.984	40.273	26.787	1.00	27.06	CPS6
ATOM	5377	CD1	ILE	90	36.410	41.147	25.584	1.00	30.06	CPS6
ATOM	5378	C	ILE	90	36.657	38.407	29.079	1.00	26.15	CPS6
ATOM	5379	O	ILE	90	36.241	39.337	29.783	1.00	25.40	CPS6
ATOM	5380	N	CYS	91	37.742	37.702	29.376	1.00	26.82	CPS6
ATOM	5381	CA	CYS	91	38.574	37.975	30.543	1.00	28.62	CPS6
ATOM	5382	CB	CYS	91	38.041	37.191	31.749	1.00	27.71	CPS6
ATOM	5383	SG	CYS	91	39.031	37.333	33.261	1.00	30.47	CPS6
ATOM	5384	C	CYS	91	39.998	37.516	30.194	1.00	29.98	CPS6
ATOM	5385	O	CYS	91	40.213	36.361	29.839	1.00	29.65	CPS6
ATOM	5386	N	THR	92	40.966	38.419	30.291	1.00	32.42	CPS6
ATOM	5387	CA	THR	92	42.344	38.078	29.948	1.00	34.14	CPS6
ATOM	5388	CB	THR	92	43.264	39.303	30.103	1.00	36.33	CPS6
ATOM	5389	OG1	THR	92	43.150	39.810	31.439	1.00	38.35	CPS6
ATOM	5390	CG2	THR	92	42.872	40.393	29.104	1.00	35.90	CPS6
ATOM	5391	C	THR	92	42.931	36.932	30.761	1.00	35.10	CPS6
ATOM	5392	O	THR	92	43.960	36.359	30.380	1.00	36.58	CPS6
ATOM	5393	N	LYS	93	42.291	36.582	31.870	1.00	33.97	CPS6
ATOM	5394	CA	LYS	93	42.808	35.503	32.698	1.00	34.28	CPS6
ATOM	5395	CB	LYS	93	42.231	35.596	34.105	1.00	35.19	CPS6
ATOM	5396	CG	LYS	93	42.654	36.867	34.827	1.00	38.98	CPS6
ATOM	5397	CD	LYS	93	42.107	36.924	36.240	1.00	40.89	CPS6
ATOM	5398	CE	LYS	93	42.416	38.263	36.898	1.00	41.92	CPS6
ATOM	5399	NZ	LYS	93	43.879	38.529	36.966	1.00	43.76	CPS6
ATOM	5400	C	LYS	93	42.575	34.111	32.126	1.00	33.08	CPS6
ATOM	5401	O	LYS	93	43.143	33.137	32.613	1.00	33.58	CPS6
ATOM	5402	N	LEU	94	41.743	34.005	31.098	1.00	31.56	CPS6
ATOM	5403	CA	LEU	94	41.489	32.702	30.487	1.00	29.96	CPS6
ATOM	5404	CB	LEU	94	40.553	31.853	31.363	1.00	31.34	CPS6
ATOM	5405	CG	LEU	94	39.321	32.481	32.035	1.00	33.01	CPS6
ATOM	5406	CD1	LEU	94	38.520	33.306	31.062	1.00	32.91	CPS6
ATOM	5407	CD2	LEU	94	38.465	31.368	32.625	1.00	35.31	CPS6
ATOM	5408	C	LEU	94	40.917	32.822	29.091	1.00	28.50	CPS6
ATOM	5409	O	LEU	94	40.531	33.909	28.654	1.00	28.02	CPS6
ATOM	5410	N	SER	95	40.861	31.692	28.398	1.00	27.95	CPS6
ATOM	5411	CA	SER	95	40.341	31.636	27.040	1.00	27.87	CPS6
ATOM	5412	CB	SER	95	40.579	30.261	26.426	1.00	28.47	CPS6
ATOM	5413	OG	SER	95	39.846	30.141	25.218	1.00	30.54	CPS6
ATOM	5414	C	SER	95	38.849	31.905	27.011	1.00	26.60	CPS6

FIG. 1A-95


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ATOM   5415  O   SER    95      38.098  31.331  27.793  1.00 25.68      CPS6
ATOM   5416  N   PRO    96      38.401  32.762  26.082  1.00 25.92      CPS6
ATOM   5417  CD  PRO    96      39.206  33.567  25.144  1.00 25.77      CPS6
ATOM   5418  CA  PRO    96      36.978  33.085  25.978  1.00 25.00      CPS6
ATOM   5419  CB  PRO    96      36.947  34.199  24.922  1.00 25.69      CPS6
ATOM   5420  CG  PRO    96      38.197  33.949  24.093  1.00 25.08      CPS6
ATOM   5421  C   PRO    96      36.129  31.873  25.602  1.00 25.28      CPS6
ATOM   5422  O   PRO    96      34.942  31.810  25.922  1.00 23.78      CPS6
ATOM   5423  N   ALA    97      36.741  30.902  24.934  1.00 24.13      CPS6
ATOM   5424  CA  ALA    97      36.023  29.701  24.534  1.00 24.78      CPS6
ATOM   5425  CB  ALA    97      36.873  28.890  23.569  1.00 25.54      CPS6
ATOM   5426  C   ALA    97      35.650  28.846  25.746  1.00 24.39      CPS6
ATOM   5427  O   ALA    97      34.783  27.980  25.657  1.00 25.77      CPS6
ATOM   5428  N   ALA    98      36.300  29.093  26.879  1.00 23.13      CPS6
ATOM   5429  CA  ALA    98      36.033  28.320  28.094  1.00 23.12      CPS6
ATOM   5430  CB  ALA    98      37.285  28.277  28.947  1.00 23.94      CPS6
ATOM   5431  C   ALA    98      34.875  28.867  28.937  1.00 23.29      CPS6
ATOM   5432  O   ALA    98      34.418  28.217  29.883  1.00 23.78      CPS6
ATOM   5433  N   VAL    99      34.398  30.055  28.593  1.00 22.50      CPS6
ATOM   5434  CA  VAL    99      33.353  30.693  29.386  1.00 22.03      CPS6
ATOM   5435  CB  VAL    99      33.776  32.130  29.747  1.00 22.74      CPS6
ATOM   5436  CG1 VAL    99      32.850  32.710  30.799  1.00 22.51      CPS6
ATOM   5437  CG2 VAL    99      35.207  32.132  30.250  1.00 24.89      CPS6
ATOM   5438  C   VAL    99      31.978  30.757  28.739  1.00 20.85      CPS6
ATOM   5439  O   VAL    99      31.850  30.969  27.534  1.00 20.38      CPS6
ATOM   5440  N   HIS   100      30.950  30.580  29.568  1.00 20.29      CPS6
ATOM   5441  CA  HIS   100      29.563  30.652  29.132  1.00 18.65      CPS6
ATOM   5442  CB  HIS   100      28.988  29.251  29.029  1.00 20.06      CPS6
ATOM   5443  CG  HIS   100      29.786  28.360  28.139  1.00 23.66      CPS6
ATOM   5444  CD2 HIS   100      30.802  27.509  28.412  1.00 26.19      CPS6
ATOM   5445  ND1 HIS   100      29.626  28.343  26.772  1.00 25.30      CPS6
ATOM   5446  CE1 HIS   100      30.511  27.518  26.239  1.00 26.78      CPS6
ATOM   5447  NE2 HIS   100      31.237  27.000  27.214  1.00 27.25      CPS6
ATOM   5448  C   HIS   100      28.806  31.440  30.186  1.00 18.48      CPS6
ATOM   5449  O   HIS   100      29.071  31.297  31.378  1.00 17.96      CPS6
ATOM   5450  N   VAL   101      27.852  32.261  29.753  1.00 17.67      CPS6
ATOM   5451  CA  VAL   101      27.092  33.060  30.697  1.00 17.87      CPS6
ATOM   5452  CB  VAL   101      27.749  34.455  30.846  1.00 19.43      CPS6
ATOM   5453  CG1 VAL   101      27.766  35.151  29.492  1.00 19.75      CPS6
ATOM   5454  CG2 VAL   101      26.984  35.314  31.860  1.00 19.30      CPS6
ATOM   5455  C   VAL   101      25.650  33.255  30.229  1.00 17.14      CPS6
ATOM   5456  O   VAL   101      25.356  33.139  29.046  1.00 16.92      CPS6
ATOM   5457  N   SER   102      24.752  33.522  31.173  1.00 17.82      CPS6
ATOM   5458  CA  SER   102      23.365  33.821  30.837  1.00 18.24      CPS6
ATOM   5459  CB  SER   102      22.450  32.592  30.926  1.00 18.94      CPS6
ATOM   5460  OG  SER   102      21.131  32.955  30.513  1.00 19.02      CPS6
ATOM   5461  C   SER   102      22.932  34.853  31.855  1.00 17.95      CPS6
ATOM   5462  O   SER   102      23.335  34.792  33.025  1.00 16.39      CPS6
ATOM   5463  N   ILE   103      22.112  35.802  31.414  1.00 16.51      CPS6
ATOM   5464  CA  ILE   103      21.630  36.864  32.291  1.00 17.17      CPS6
ATOM   5465  CB  ILE   103      22.243  38.240  31.884  1.00 17.60      CPS6
ATOM   5466  CG2 ILE   103      21.761  39.341  32.845  1.00 19.81      CPS6
ATOM   5467  CG1 ILE   103      23.769  38.152  31.899  1.00 19.89      CPS6
ATOM   5468  CD1 ILE   103      24.483  39.402  31.357  1.00 19.80      CPS6
ATOM   5469  C   ILE   103      20.112  36.933  32.131  1.00 17.69      CPS6
ATOM   5470  O   ILE   103      19.595  36.760  31.021  1.00 17.52      CPS6
ATOM   5471  N   THR   104      19.414  37.173  33.237  1.00 18.18      CPS6
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FIG. 1A-96

ATOM	5472	CA	THR	104	17.954	37.283	33.226	1.00 18.92	CPS6
ATOM	5473	CB	THR	104	17.285	35.948	33.660	1.00 20.47	CPS6
ATOM	5474	OG1	THR	104	15.864	36.026	33.456	1.00 20.23	CPS6
ATOM	5475	CG2	THR	104	17.578	35.648	35.130	1.00 17.86	CPS6
ATOM	5476	C	THR	104	17.523	38.429	34.159	1.00 20.41	CPS6
ATOM	5477	O	THR	104	18.306	38.901	34.990	1.00 19.19	CPS6
ATOM	5478	N	HIS	105	16.280	38.880	34.001	1.00 21.31	CPS6
ATOM	5479	CA	HIS	105	15.751	39.984	34.799	1.00 22.86	CPS6
ATOM	5480	CB	HIS	105	15.802	41.299	33.998	1.00 26.24	CPS6
ATOM	5481	CG	HIS	105	17.175	41.721	33.578	1.00 30.59	CPS6
ATOM	5482	CD2	HIS	105	17.889	41.444	32.461	1.00 32.14	CPS6
ATOM	5483	ND1	HIS	105	17.974	42.534	34.355	1.00 33.04	CPS6
ATOM	5484	CE1	HIS	105	19.122	42.739	33.733	1.00 33.19	CPS6
ATOM	5485	NE2	HIS	105	19.097	42.089	32.582	1.00 32.49	CPS6
ATOM	5486	C	HIS	105	14.278	39.762	35.129	1.00 23.27	CPS6
ATOM	5487	O	HIS	105	13.575	39.039	34.417	1.00 21.93	CPS6
ATOM	5488	N	THR	106	13.837	40.393	36.212	1.00 23.40	CPS6
ATOM	5489	CA	THR	106	12.430	40.421	36.605	1.00 25.56	CPS6
ATOM	5490	CB	THR	106	12.067	39.537	37.816	1.00 27.06	CPS6
ATOM	5491	OG1	THR	106	12.664	40.059	39.015	1.00 26.80	CPS6
ATOM	5492	CG2	THR	106	12.496	38.102	37.567	1.00 25.79	CPS6
ATOM	5493	C	THR	106	12.266	41.879	37.013	1.00 27.51	CPS6
ATOM	5494	O	THR	106	13.230	42.651	36.964	1.00 26.39	CPS6
ATOM	5495	N	LYS	107	11.069	42.272	37.423	1.00 28.29	CPS6
ATOM	5496	CA	LYS	107	10.880	43.662	37.810	1.00 29.88	CPS6
ATOM	5497	CB	LYS	107	9.440	43.899	38.268	1.00 32.33	CPS6
ATOM	5498	CG	LYS	107	9.155	45.357	38.599	1.00 36.25	CPS6
ATOM	5499	CD	LYS	107	7.745	45.549	39.147	1.00 39.84	CPS6
ATOM	5500	CE	LYS	107	7.473	47.024	39.442	1.00 41.42	CPS6
ATOM	5501	NZ	LYS	107	6.102	47.246	39.995	1.00 45.05	CPS6
ATOM	5502	C	LYS	107	11.839	44.132	38.905	1.00 29.50	CPS6
ATOM	5503	O	LYS	107	12.367	45.243	38.823	1.00 29.28	CPS6
ATOM	5504	N	GLU	108	12.081	43.289	39.912	1.00 27.21	CPS6
ATOM	5505	CA	GLU	108	12.945	43.667	41.033	1.00 26.33	CPS6
ATOM	5506	CB	GLU	108	12.239	43.363	42.358	1.00 30.27	CPS6
ATOM	5507	CG	GLU	108	10.841	43.953	42.480	1.00 36.27	CPS6
ATOM	5508	CD	GLU	108	10.259	43.782	43.874	1.00 41.02	CPS6
ATOM	5509	OE1	GLU	108	10.158	42.632	44.354	1.00 44.74	CPS6
ATOM	5510	OE2	GLU	108	9.897	44.803	44.497	1.00 45.09	CPS6
ATOM	5511	C	GLU	108	14.333	43.033	41.108	1.00 25.31	CPS6
ATOM	5512	O	GLU	108	15.145	43.437	41.936	1.00 22.62	CPS6
ATOM	5513	N	TYR	109	14.609	42.043	40.266	1.00 22.54	CPS6
ATOM	5514	CA	TYR	109	15.900	41.368	40.333	1.00 22.99	CPS6
ATOM	5515	CB	TYR	109	15.728	39.954	40.909	1.00 22.64	CPS6
ATOM	5516	CG	TYR	109	15.175	39.906	42.310	1.00 24.37	CPS6
ATOM	5517	CD1	TYR	109	15.988	40.167	43.411	1.00 24.51	CPS6
ATOM	5518	CE1	TYR	109	15.465	40.190	44.701	1.00 26.40	CPS6
ATOM	5519	CD2	TYR	109	13.821	39.661	42.531	1.00 24.67	CPS6
ATOM	5520	CE2	TYR	109	13.286	39.683	43.809	1.00 24.88	CPS6
ATOM	5521	CZ	TYR	109	14.106	39.946	44.884	1.00 26.56	CPS6
ATOM	5522	OH	TYR	109	13.576	39.968	46.144	1.00 29.07	CPS6
ATOM	5523	C	TYR	109	16.609	41.211	39.008	1.00 21.70	CPS6
ATOM	5524	O	TYR	109	15.993	41.280	37.945	1.00 22.54	CPS6
ATOM	5525	N	ALA	110	17.926	41.012	39.103	1.00 21.84	CPS6
ATOM	5526	CA	ALA	110	18.770	40.702	37.950	1.00 20.16	CPS6
ATOM	5527	CB	ALA	110	19.785	41.803	37.666	1.00 21.73	CPS6
ATOM	5528	C	ALA	110	19.492	39.445	38.443	1.00 20.44	CPS6

FIG. 1A-97

ATOM	5529	O	ALA	110	19.824	39.345	39.621	1.00	21.38	CPS6
ATOM	5530	N	ALA	111	19.714	38.476	37.560	1.00	19.56	CPS6
ATOM	5531	CA	ALA	111	20.415	37.272	37.962	1.00	17.92	CPS6
ATOM	5532	CB	ALA	111	19.410	36.180	38.358	1.00	18.78	CPS6
ATOM	5533	C	ALA	111	21.286	36.791	36.808	1.00	18.10	CPS6
ATOM	5534	O	ALA	111	21.044	37.114	35.654	1.00	19.16	CPS6
ATOM	5535	N	ALA	112	22.319	36.033	37.128	1.00	18.13	CPS6
ATOM	5536	CA	ALA	112	23.175	35.509	36.083	1.00	18.42	CPS6
ATOM	5537	CB	ALA	112	24.206	36.565	35.659	1.00	16.42	CPS6
ATOM	5538	C	ALA	112	23.882	34.260	36.569	1.00	17.57	CPS6
ATOM	5539	O	ALA	112	24.000	34.017	37.778	1.00	18.87	CPS6
ATOM	5540	N	GLN	113	24.327	33.449	35.619	1.00	17.13	CPS6
ATOM	5541	CA	GLN	113	25.065	32.247	35.971	1.00	17.77	CPS6
ATOM	5542	CB	GLN	113	24.163	31.017	35.898	1.00	19.54	CPS6
ATOM	5543	CG	GLN	113	23.699	30.693	34.495	1.00	21.95	CPS6
ATOM	5544	CD	GLN	113	22.787	29.472	34.435	1.00	25.73	CPS6
ATOM	5545	OE1	GLN	113	22.446	29.002	33.352	1.00	27.72	CPS6
ATOM	5546	NE2	GLN	113	22.378	28.968	35.594	1.00	27.67	CPS6
ATOM	5547	C	GLN	113	26.205	32.133	34.968	1.00	16.69	CPS6
ATOM	5548	O	GLN	113	26.104	32.622	33.840	1.00	16.20	CPS6
ATOM	5549	N	VAL	114	27.288	31.499	35.391	1.00	17.22	CPS6
ATOM	5550	CA	VAL	114	28.449	31.324	34.535	1.00	17.47	CPS6
ATOM	5551	CB	VAL	114	29.605	32.300	34.948	1.00	17.72	CPS6
ATOM	5552	CG1	VAL	114	30.931	31.901	34.243	1.00	16.56	CPS6
ATOM	5553	CG2	VAL	114	29.222	33.738	34.581	1.00	17.27	CPS6
ATOM	5554	C	VAL	114	28.964	29.911	34.693	1.00	18.72	CPS6
ATOM	5555	O	VAL	114	28.880	29.338	35.776	1.00	19.21	CPS6
ATOM	5556	N	VAL	115	29.461	29.338	33.604	1.00	18.94	CPS6
ATOM	5557	CA	VAL	115	30.090	28.027	33.684	1.00	19.93	CPS6
ATOM	5558	CB	VAL	115	29.311	26.916	32.928	1.00	19.40	CPS6
ATOM	5559	CG1	VAL	115	30.143	25.631	32.901	1.00	20.42	CPS6
ATOM	5560	CG2	VAL	115	27.981	26.638	33.628	1.00	19.61	CPS6
ATOM	5561	C	VAL	115	31.453	28.231	33.023	1.00	20.14	CPS6
ATOM	5562	O	VAL	115	31.562	28.860	31.958	1.00	19.69	CPS6
ATOM	5563	N	ILE	116	32.498	27.750	33.680	1.00	19.47	CPS6
ATOM	5564	CA	ILE	116	33.839	27.853	33.121	1.00	21.42	CPS6
ATOM	5565	CB	ILE	116	34.806	28.617	34.068	1.00	21.08	CPS6
ATOM	5566	CG2	ILE	116	36.235	28.577	33.505	1.00	23.06	CPS6
ATOM	5567	CG1	ILE	116	34.365	30.082	34.195	1.00	21.71	CPS6
ATOM	5568	CD1	ILE	116	35.180	30.906	35.213	1.00	21.07	CPS6
ATOM	5569	C	ILE	116	34.320	26.420	32.940	1.00	24.10	CPS6
ATOM	5570	O	ILE	116	34.264	25.615	33.872	1.00	23.26	CPS6
ATOM	5571	N	GLU	117	34.759	26.103	31.731	1.00	25.26	CPS6
ATOM	5572	CA	GLU	117	35.243	24.769	31.424	1.00	29.11	CPS6
ATOM	5573	CB	GLU	117	34.878	24.369	30.001	1.00	30.47	CPS6
ATOM	5574	CG	GLU	117	33.446	24.548	29.587	1.00	33.45	CPS6
ATOM	5575	CD	GLU	117	33.226	24.007	28.194	1.00	36.82	CPS6
ATOM	5576	OE1	GLU	117	33.345	22.776	28.022	1.00	39.37	CPS6
ATOM	5577	OE2	GLU	117	32.959	24.804	27.271	1.00	38.14	CPS6
ATOM	5578	C	GLU	117	36.754	24.698	31.503	1.00	31.19	CPS6
ATOM	5579	O	GLU	117	37.445	25.712	31.392	1.00	28.72	CPS6
ATOM	5580	N	ARG	118	37.259	23.484	31.686	1.00	34.06	CPS6
ATOM	5581	CA	ARG	118	38.692	23.267	31.686	1.00	39.18	CPS6
ATOM	5582	CB	ARG	118	39.089	22.180	32.703	1.00	40.91	CPS6
ATOM	5583	CG	ARG	118	38.327	20.872	32.574	1.00	46.37	CPS6
ATOM	5584	CD	ARG	118	38.840	19.776	33.528	1.00	49.12	CPS6
ATOM	5585	NE	ARG	118	38.479	19.996	34.930	1.00	50.78	CPS6

FIG. 1A-98

ATOM	5586	CZ	ARG	118	39.095	20.849	35.744	1.00	51.80	CPS6
ATOM	5587	NH1	ARG	118	40.113	21.575	35.304	1.00	53.03	CPS6
ATOM	5588	NH2	ARG	118	38.692	20.977	37.003	1.00	51.56	CPS6
ATOM	5589	C	ARG	118	38.895	22.789	30.250	1.00	40.50	CPS6
ATOM	5590	O	ARG	118	38.365	21.750	29.862	1.00	41.56	CPS6
ATOM	5591	N	LEU	119	39.615	23.562	29.445	1.00	42.65	CPS6
ATOM	5592	CA	LEU	119	39.833	23.176	28.055	1.00	44.91	CPS6
ATOM	5593	CB	LEU	119	40.106	24.414	27.196	1.00	45.15	CPS6
ATOM	5594	CG	LEU	119	38.970	25.432	27.070	1.00	45.37	CPS6
ATOM	5595	CD1	LEU	119	39.442	26.618	26.246	1.00	44.17	CPS6
ATOM	5596	CD2	LEU	119	37.752	24.776	26.427	1.00	45.02	CPS6
ATOM	5597	C	LEU	119	40.991	22.193	27.918	1.00	46.41	CPS6
ATOM	5598	OT1	LEU	119	41.823	22.138	28.848	1.00	47.25	CPS6
ATOM	5599	OT2	LEU	119	41.055	21.501	26.874	1.00	47.76	CPS6
ATOM	5600	O	HOH	1	74.183	58.190	-19.320	1.00	16.24	AT
ATOM	5601	O	HOH	2	50.451	28.498	2.245	1.00	16.26	AT
ATOM	5602	O	HOH	3	72.513	43.845	5.247	1.00	16.95	AT
ATOM	5603	O	HOH	4	59.768	49.591	13.381	1.00	18.99	AT
ATOM	5604	O	HOH	5	9.919	40.963	40.359	1.00	17.22	AT
ATOM	5605	O	HOH	6	57.301	49.721	15.536	1.00	18.51	AT
ATOM	5606	O	HOH	7	72.254	36.424	22.184	1.00	19.44	AT
ATOM	5607	O	HOH	8	15.486	40.288	48.189	1.00	19.00	AT
ATOM	5608	O	HOH	9	22.359	26.422	33.132	1.00	28.69	AT
ATOM	5609	O	HOH	10	62.648	41.000	12.765	1.00	26.69	AT
ATOM	5610	O	HOH	11	27.253	11.532	60.836	1.00	33.03	AT
ATOM	5611	O	HOH	12	4.545	29.482	16.753	1.00	34.49	AT
ATOM	5612	O	HOH	13	14.678	33.346	17.568	1.00	28.16	AT
ATOM	5613	O	HOH	14	2.443	17.966	21.642	1.00	31.50	AT
ATOM	5614	O	HOH	15	13.387	44.897	46.109	1.00	36.84	AT
ATOM	5615	O	HOH	16	64.048	43.971	9.189	1.00	27.36	AT
ATOM	5616	O	HOH	17	17.153	29.081	61.693	1.00	38.80	AT
ATOM	5617	O	HOH	18	15.565	11.097	37.041	1.00	32.04	AT
ATOM	5618	O	HOH	19	66.736	39.802	9.758	1.00	31.88	AT
ATOM	5619	O	HOH	20	68.806	35.163	19.609	1.00	43.12	AT
ATOM	5620	O	HOH	21	28.442	30.448	25.270	1.00	35.30	AT
ATOM	5621	O	HOH	22	20.356	37.769	28.103	1.00	40.41	AT
ATOM	5622	O	HOH	23	27.784	56.284	42.007	1.00	39.44	AT
ATOM	5623	O	HOH	24	9.819	21.853	51.711	1.00	48.93	AT
ATOM	5624	O	HOH	25	18.794	48.571	49.608	1.00	38.44	AT
ATOM	5625	O	HOH	26	50.953	43.970	28.198	1.00	29.58	AT
ATOM	5626	O	HOH	27	22.120	28.021	18.001	1.00	41.70	AT
ATOM	5627	O	HOH	28	18.224	7.825	50.971	1.00	37.65	AT
ATOM	5628	O	HOH	29	45.010	40.785	1.909	1.00	35.18	AT
ATOM	5629	O	HOH	30	64.211	31.229	23.988	1.00	42.82	AT
ATOM	5630	O	HOH	31	55.673	59.846	2.934	1.00	40.75	AT
ATOM	5631	O	HOH	32	12.144	16.656	71.990	1.00	45.41	AT
ATOM	5632	O	HOH	33	26.174	28.070	35.889	1.00	33.23	AT
ATOM	5633	O	HOH	34	23.423	24.108	37.385	1.00	33.85	AT
ATOM	5634	O	HOH	35	72.206	58.375	9.452	1.00	45.41	AT
ATOM	5635	O	HOH	36	4.583	28.820	43.211	1.00	37.91	AT
ATOM	5636	O	HOH	37	54.428	31.469	26.691	1.00	40.61	AT
ATOM	5637	O	HOH	38	5.129	39.360	42.159	1.00	34.31	AT
ATOM	5638	O	HOH	39	61.288	9.543	3.422	1.00	45.78	AT
ATOM	5639	O	HOH	40	41.144	21.554	50.056	1.00	46.77	AT
ATOM	5640	O	HOH	41	45.899	31.375	23.218	1.00	36.69	AT
ATOM	5641	O	HOH	42	46.684	40.019	4.072	1.00	40.88	AT
ATOM	5642	O	HOH	43	32.060	30.436	24.972	1.00	38.00	AT

FIG. 1A-99

ATOM	5643	O	HOH	44	27.193	55.260	39.276	1.00	39.83	AT
ATOM	5644	O	HOH	45	74.083	12.016	10.419	1.00	37.57	AT
ATOM	5645	O	HOH	46	7.161	11.806	20.918	1.00	37.74	AT
ATOM	5646	O	HOH	47	37.597	37.224	10.717	1.00	44.06	AT
ATOM	5647	O	HOH	48	26.713	40.428	46.123	1.00	47.01	AT
ATOM	5648	O	HOH	49	73.327	31.524	18.039	1.00	39.95	AT
ATOM	5649	O	HOH	50	6.885	35.701	48.910	1.00	38.11	AT
ATOM	5650	O	HOH	51	12.147	30.555	62.867	1.00	45.67	AT
ATOM	5651	O	HOH	52	45.035	35.126	28.209	1.00	45.09	AT
ATOM	5652	O	HOH	53	45.816	30.463	0.531	1.00	37.06	AT
ATOM	5653	O	HOH	54	37.959	49.546	12.787	1.00	41.97	AT
ATOM	5654	O	HOH	55	29.307	59.252	40.586	1.00	54.29	AT
ATOM	5655	O	HOH	56	33.064	30.245	14.482	1.00	53.18	AT
ATOM	5656	O	HOH	57	5.959	29.404	40.923	1.00	42.88	AT
ATOM	5657	O	HOH	58	72.015	56.594	2.111	1.00	41.98	AT
ATOM	5658	O	HOH	59	34.149	9.199	46.267	1.00	42.25	AT
ATOM	5659	O	HOH	60	56.871	24.901	5.890	1.00	43.48	AT
ATOM	5660	O	HOH	61	53.366	27.278	27.533	1.00	46.43	AT
ATOM	5661	O	HOH	62	51.684	37.046	30.830	1.00	46.25	AT
ATOM	5662	O	HOH	63	52.569	48.531	8.124	1.00	42.45	AT
ATOM	5663	O	HOH	64	19.990	15.518	32.236	1.00	48.76	AT
ATOM	5664	O	HOH	65	64.540	44.979	26.386	1.00	42.49	AT
ATOM	5665	O	HOH	66	30.220	13.054	46.228	1.00	52.13	AT
ATOM	5666	O	HOH	67	54.239	52.985	1.438	1.00	45.12	AT
ATOM	5667	O	HOH	68	20.023	54.748	37.127	1.00	39.76	AT
ATOM	5668	O	HOH	69	8.456	21.336	37.515	1.00	48.76	AT
ATOM	5669	O	HOH	70	35.909	45.522	2.599	1.00	46.39	AT
ATOM	5670	O	HOH	71	53.886	30.997	19.731	1.00	43.92	AT
ATOM	5671	O	HOH	72	10.033	24.488	66.210	1.00	53.66	AT
ATOM	5672	O	HOH	73	58.903	57.250	13.037	1.00	41.23	AT
ATOM	5673	O	HOH	74	62.777	15.875	1.984	1.00	41.20	AT
ATOM	5674	O	HOH	75	42.217	40.323	33.742	1.00	43.11	AT
ATOM	5675	O	HOH	76	20.956	40.692	29.179	1.00	49.81	AT
ATOM	5676	O	HOH	77	46.166	43.977	11.730	1.00	36.26	AT
ATOM	5677	O	HOH	78	66.744	59.058	16.145	1.00	56.18	AT
ATOM	5678	O	HOH	79	45.851	25.881	4.391	1.00	55.88	AT
ATOM	5679	O	HOH	80	75.174	49.183	6.063	1.00	47.74	AT
ATOM	5680	O	HOH	81	29.310	41.802	17.220	1.00	55.92	AT
ATOM	5681	O	HOH	82	1.927	35.649	42.778	1.00	51.25	AT
ATOM	5682	O	HOH	83	-1.663	38.805	38.155	1.00	39.95	AT
ATOM	5683	O	HOH	84	14.052	11.606	52.410	1.00	45.64	AT
ATOM	5684	O	HOH	85	12.374	37.222	15.756	1.00	49.24	AT
ATOM	5685	O	HOH	86	31.903	41.930	45.468	1.00	45.19	AT
ATOM	5686	O	HOH	87	33.483	20.380	56.292	1.00	53.83	AT
ATOM	5687	O	HOH	88	74.639	45.461	5.020	1.00	41.59	AT
ATOM	5688	O	HOH	89	37.028	19.108	53.278	1.00	43.77	AT
ATOM	5689	O	HOH	90	38.593	49.011	6.342	1.00	51.49	AT
ATOM	5690	O	HOH	91	52.402	56.617	3.593	1.00	53.57	AT
ATOM	5691	O	HOH	92	5.772	28.675	61.930	1.00	44.14	AT
ATOM	5692	O	HOH	93	32.173	36.302	19.628	1.00	45.70	AT
ATOM	5693	O	HOH	94	52.026	42.123	29.953	1.00	47.73	AT
ATOM	5694	O	HOH	95	47.042	40.027	29.849	1.00	57.66	AT
ATOM	5695	O	HOH	96	62.041	43.614	30.370	1.00	49.31	AT
ATOM	5696	O	HOH	97	61.630	30.997	18.476	1.00	53.79	AT
ATOM	5697	O	HOH	98	11.168	13.661	45.409	1.00	45.46	AT
ATOM	5698	O	HOH	99	28.738	15.678	20.064	1.00	63.95	AT
ATOM	5699	O	HOH	100	37.162	57.858	42.839	1.00	49.29	AT

FIG. 1A-100

ATOM	5700	O	HOH	101	56.970	48.398	18.183	1.00	20.07	AT
ATOM	5701	O	HOH	102	16.747	17.196	32.059	1.00	21.58	AT
ATOM	5702	O	HOH	103	45.835	52.603	17.631	1.00	19.92	AT
ATOM	5703	O	HOH	104	-5.526	20.298	17.919	1.00	20.40	AT
ATOM	5704	O	HOH	105	16.573	18.225	29.320	1.00	21.11	AT
ATOM	5705	O	HOH	106	28.084	33.122	26.572	1.00	21.96	AT
ATOM	5706	O	HOH	107	56.776	49.897	20.691	1.00	20.77	AT
ATOM	5707	O	HOH	108	61.822	31.586	15.608	1.00	22.44	AT
ATOM	5708	O	HOH	109	75.499	25.254	21.262	1.00	22.49	AT
ATOM	5709	O	HOH	110	52.716	36.178	-8.615	1.00	23.96	AT
ATOM	5710	O	HOH	111	30.657	33.717	27.675	1.00	22.13	AT
ATOM	5711	O	HOH	112	31.857	23.322	43.883	1.00	22.91	AT
ATOM	5712	O	HOH	113	16.560	16.176	27.250	1.00	22.50	AT
ATOM	5713	O	HOH	114	48.919	55.521	18.754	1.00	22.71	AT
ATOM	5714	O	HOH	115	30.469	45.806	26.160	1.00	24.06	AT
ATOM	5715	O	HOH	116	29.611	29.912	44.889	1.00	23.26	AT
ATOM	5716	O	HOH	117	14.658	45.605	43.596	1.00	25.77	AT
ATOM	5717	O	HOH	118	38.482	35.704	27.602	1.00	23.84	AT
ATOM	5718	O	HOH	119	33.048	33.856	26.010	1.00	23.17	AT
ATOM	5719	O	HOH	120	11.956	35.757	52.609	1.00	26.32	AT
ATOM	5720	O	HOH	121	72.585	45.998	2.976	1.00	23.39	AT
ATOM	5721	O	HOH	122	45.040	32.707	1.982	1.00	25.55	AT
ATOM	5722	O	HOH	123	71.609	48.727	2.944	1.00	24.67	AT
ATOM	5723	O	HOH	124	34.369	7.558	43.913	1.00	24.87	AT
ATOM	5724	O	HOH	125	4.595	36.818	41.429	1.00	25.98	AT
ATOM	5725	O	HOH	126	11.206	23.871	43.608	1.00	25.23	AT
ATOM	5726	O	HOH	127	14.284	14.636	65.129	1.00	25.02	AT
ATOM	5727	O	HOH	128	70.983	32.077	16.439	1.00	25.53	AT
ATOM	5728	O	HOH	129	15.935	10.066	59.658	1.00	25.84	AT
ATOM	5729	O	HOH	130	17.042	11.420	57.203	1.00	25.22	AT
ATOM	5730	O	HOH	131	78.508	30.572	16.070	1.00	25.80	AT
ATOM	5731	O	HOH	132	31.882	25.438	41.276	1.00	25.44	AT
ATOM	5732	O	HOH	133	68.333	21.576	13.174	1.00	27.25	AT
ATOM	5733	O	HOH	134	59.808	51.543	15.137	1.00	26.71	AT
ATOM	5734	O	HOH	135	51.803	45.823	2.829	1.00	28.23	AT
ATOM	5735	O	HOH	136	23.948	33.437	19.543	1.00	26.93	AT
ATOM	5736	O	HOH	137	77.529	24.686	-0.187	1.00	27.06	AT
ATOM	5737	O	HOH	138	36.414	47.961	27.068	1.00	26.59	AT
ATOM	5738	O	HOH	139	15.210	37.727	30.916	1.00	26.63	AT
ATOM	5739	O	HOH	140	26.736	13.803	59.642	1.00	27.51	AT
ATOM	5740	O	HOH	141	59.707	29.029	-5.923	1.00	28.00	AT
ATOM	5741	O	HOH	142	73.385	50.907	2.916	1.00	25.70	AT
ATOM	5742	O	HOH	143	25.372	31.413	54.764	1.00	28.23	AT
ATOM	5743	O	HOH	144	8.726	40.753	36.473	1.00	28.04	AT
ATOM	5744	O	HOH	145	21.631	52.226	39.835	1.00	27.68	AT
ATOM	5745	O	HOH	146	6.966	31.512	19.584	1.00	26.22	AT
ATOM	5746	O	HOH	147	33.568	23.343	41.390	1.00	28.59	AT
ATOM	5747	O	HOH	148	47.104	33.497	24.474	1.00	31.57	AT
ATOM	5748	O	HOH	149	42.706	46.788	25.123	1.00	28.27	AT
ATOM	5749	O	HOH	150	15.361	13.776	53.744	1.00	28.43	AT
ATOM	5750	O	HOH	151	49.210	27.704	6.023	1.00	26.48	AT
ATOM	5751	O	HOH	152	69.742	37.893	23.208	1.00	28.63	AT
ATOM	5752	O	HOH	153	62.896	46.941	28.207	1.00	29.51	AT
ATOM	5753	O	HOH	154	66.194	34.304	-2.754	1.00	27.04	AT
ATOM	5754	O	HOH	155	56.380	56.783	12.351	1.00	29.49	AT
ATOM	5755	O	HOH	156	62.810	23.721	9.697	1.00	29.08	AT
ATOM	5756	O	HOH	157	59.600	48.626	-20.735	1.00	30.39	AT

FIG. 1A-101

ATOM	5757	O	HOH	158	63.447	33.873	17.572	1.00	29.71	AT
ATOM	5758	O	HOH	159	11.724	13.599	66.211	1.00	27.82	AT
ATOM	5759	O	HOH	160	60.558	22.006	10.718	1.00	28.85	AT
ATOM	5760	O	HOH	161	46.499	54.700	19.899	1.00	29.19	AT
ATOM	5761	O	HOH	162	63.410	57.441	-12.830	1.00	29.14	AT
ATOM	5762	O	HOH	163	16.531	13.383	27.915	1.00	29.15	AT
ATOM	5763	O	HOH	164	57.094	58.123	-5.057	1.00	30.67	AT
ATOM	5764	O	HOH	165	55.029	24.601	-1.884	1.00	27.07	AT
ATOM	5765	O	HOH	166	13.338	35.151	24.133	1.00	28.54	AT
ATOM	5766	O	HOH	167	35.398	47.783	6.493	1.00	28.26	AT
ATOM	5767	O	HOH	168	70.174	56.885	-10.515	1.00	31.78	AT
ATOM	5768	O	HOH	169	25.901	44.946	25.667	1.00	31.94	AT
ATOM	5769	O	HOH	170	50.393	53.846	23.119	1.00	28.26	AT
ATOM	5770	O	HOH	171	62.156	25.716	13.450	1.00	31.00	AT
ATOM	5771	O	HOH	172	42.474	44.185	26.823	1.00	31.95	AT
ATOM	5772	O	HOH	173	77.820	49.020	-5.810	1.00	32.32	AT
ATOM	5773	O	HOH	174	67.420	39.148	-19.340	1.00	29.68	AT
ATOM	5774	O	HOH	175	48.791	40.644	-3.702	1.00	28.90	AT
ATOM	5775	O	HOH	176	33.117	16.234	43.002	1.00	31.48	AT
ATOM	5776	O	HOH	177	15.122	24.092	63.819	1.00	30.47	AT
ATOM	5777	O	HOH	178	64.991	30.299	-1.464	1.00	30.76	AT
ATOM	5778	O	HOH	179	15.212	16.862	21.098	1.00	32.61	AT
ATOM	5779	O	HOH	180	8.026	30.440	48.746	1.00	29.36	AT
ATOM	5780	O	HOH	181	15.063	29.611	60.193	1.00	29.52	AT
ATOM	5781	O	HOH	182	-4.236	31.973	27.775	1.00	33.07	AT
ATOM	5782	O	HOH	183	41.379	28.581	29.607	1.00	31.08	AT
ATOM	5783	O	HOH	184	30.685	20.525	44.633	1.00	30.33	AT
ATOM	5784	O	HOH	185	25.786	35.845	47.678	1.00	31.51	AT
ATOM	5785	O	HOH	186	33.235	47.941	17.895	1.00	29.68	AT
ATOM	5786	O	HOH	187	64.882	30.921	17.515	1.00	30.10	AT
ATOM	5787	O	HOH	188	5.685	13.963	30.264	1.00	32.30	AT
ATOM	5788	O	HOH	189	-4.735	20.413	39.978	1.00	33.19	AT
ATOM	5789	O	HOH	190	44.587	45.272	8.578	1.00	31.21	AT
ATOM	5790	O	HOH	191	57.838	12.743	11.965	1.00	31.57	AT
ATOM	5791	O	HOH	192	16.393	22.844	66.100	1.00	34.23	AT
ATOM	5792	O	HOH	193	4.372	22.943	37.792	1.00	32.96	AT
ATOM	5793	O	HOH	194	71.929	20.305	14.473	1.00	32.09	AT
ATOM	5794	O	HOH	195	28.925	15.553	59.281	1.00	30.49	AT
ATOM	5795	O	HOH	196	53.796	25.895	-4.052	1.00	33.01	AT
ATOM	5796	O	HOH	197	6.468	23.780	36.296	1.00	34.02	AT
ATOM	5797	O	HOH	198	53.710	44.972	-1.506	1.00	33.84	AT
ATOM	5798	O	HOH	199	19.319	42.034	48.498	1.00	31.81	AT
ATOM	5799	O	HOH	200	24.603	12.893	57.779	1.00	32.45	AT
ATOM	5800	O	HOH	201	82.186	45.693	-2.681	1.00	34.17	AT
ATOM	5801	O	HOH	202	11.264	18.716	60.799	1.00	36.53	AT
ATOM	5802	O	HOH	203	79.085	17.668	9.255	1.00	31.67	AT
ATOM	5803	O	HOH	204	59.866	52.931	11.834	1.00	30.91	AT
ATOM	5804	O	HOH	205	13.907	16.278	62.855	1.00	36.18	AT
ATOM	5805	O	HOH	206	16.412	14.129	56.660	1.00	32.42	AT
ATOM	5806	O	HOH	207	66.234	40.890	-9.847	1.00	31.86	AT
ATOM	5807	O	HOH	208	10.481	11.237	25.068	1.00	32.03	AT
ATOM	5808	O	HOH	209	5.289	19.707	30.585	1.00	33.17	AT
ATOM	5809	O	HOH	210	39.446	40.017	23.668	1.00	33.18	AT
ATOM	5810	O	HOH	211	54.509	23.461	6.035	1.00	35.31	AT
ATOM	5811	O	HOH	212	51.401	31.567	11.354	1.00	32.75	AT
ATOM	5812	O	HOH	213	28.205	23.736	55.152	1.00	30.83	AT
ATOM	5813	O	HOH	214	50.324	34.946	-7.659	1.00	34.98	AT

FIG. 1A-102

ATOM	5814	O	HOH	215	30.129	20.719	56.661	1.00	32.37	AT
ATOM	5815	O	HOH	216	58.457	50.516	-18.849	1.00	32.27	AT
ATOM	5816	O	HOH	217	44.476	34.908	24.562	1.00	35.00	AT
ATOM	5817	O	HOH	218	9.990	35.693	24.724	1.00	34.96	AT
ATOM	5818	O	HOH	219	11.096	35.811	32.093	1.00	34.27	AT
ATOM	5819	O	HOH	220	12.913	17.730	46.309	1.00	34.71	AT
ATOM	5820	O	HOH	221	65.231	44.053	-7.852	1.00	32.99	AT
ATOM	5821	O	HOH	222	38.789	35.275	9.625	1.00	34.60	AT
ATOM	5822	O	HOH	223	12.929	25.623	47.543	1.00	32.40	AT
ATOM	5823	O	HOH	224	74.529	33.737	18.589	1.00	33.85	AT
ATOM	5824	O	HOH	225	16.279	43.522	36.165	1.00	33.82	AT
ATOM	5825	O	HOH	226	13.480	14.423	55.667	1.00	35.36	AT
ATOM	5826	O	HOH	227	4.656	17.272	27.720	1.00	34.90	AT
ATOM	5827	O	HOH	228	55.566	43.939	-14.228	1.00	37.00	AT
ATOM	5828	O	HOH	229	18.454	21.396	68.984	1.00	35.96	AT
ATOM	5829	O	HOH	230	56.014	51.348	-16.697	1.00	37.91	AT
ATOM	5830	O	HOH	231	71.572	46.002	-9.177	1.00	36.91	AT
ATOM	5831	O	HOH	232	39.465	30.116	20.475	1.00	46.92	AT
ATOM	5832	O	HOH	233	40.113	37.155	25.795	1.00	31.64	AT
ATOM	5833	O	HOH	234	14.226	44.782	35.447	1.00	33.52	AT
ATOM	5834	O	HOH	235	20.027	45.208	30.512	1.00	33.92	AT
ATOM	5835	O	HOH	236	61.895	17.484	0.210	1.00	36.39	AT
ATOM	5836	O	HOH	237	26.769	18.525	65.425	1.00	33.45	AT
ATOM	5837	O	HOH	238	30.216	49.429	23.557	1.00	38.87	AT
ATOM	5838	O	HOH	239	12.005	18.680	49.514	1.00	35.80	AT
ATOM	5839	O	HOH	240	40.174	39.987	26.354	1.00	36.59	AT
ATOM	5840	O	HOH	241	19.654	14.821	28.728	1.00	35.91	AT
ATOM	5841	O	HOH	242	55.447	29.046	11.959	1.00	36.10	AT
ATOM	5842	O	HOH	243	67.323	29.753	-3.238	1.00	39.47	AT
ATOM	5843	O	HOH	244	84.687	32.541	17.389	1.00	39.50	AT
ATOM	5844	O	HOH	245	54.503	28.663	-6.976	1.00	36.28	AT
ATOM	5845	O	HOH	246	35.636	37.561	8.625	1.00	41.11	AT
ATOM	5846	O	HOH	247	10.020	25.331	46.396	1.00	38.25	AT
ATOM	5847	O	HOH	248	11.151	27.733	14.203	1.00	38.20	AT
ATOM	5848	O	HOH	249	10.978	20.075	53.913	1.00	37.44	AT
ATOM	5849	O	HOH	250	77.340	21.792	0.783	1.00	40.63	AT
ATOM	5850	O	HOH	251	63.681	23.994	15.360	1.00	37.38	AT
ATOM	5851	O	HOH	252	11.477	23.218	48.380	1.00	37.57	AT
ATOM	5852	O	HOH	253	24.484	40.133	44.556	1.00	37.00	AT
ATOM	5853	O	HOH	254	26.870	34.997	63.642	1.00	37.28	AT
ATOM	5854	O	HOH	255	38.821	41.107	28.862	1.00	37.55	AT
ATOM	5855	O	HOH	256	17.119	53.559	27.111	1.00	35.75	AT
ATOM	5856	O	HOH	257	31.732	49.464	21.724	1.00	40.71	AT
ATOM	5857	O	HOH	258	37.233	48.595	24.778	1.00	37.38	AT
ATOM	5858	O	HOH	259	64.957	31.599	-4.165	1.00	34.72	AT
ATOM	5859	O	HOH	260	42.059	35.767	26.985	1.00	38.69	AT
ATOM	5860	O	HOH	261	53.170	52.497	-1.737	1.00	41.39	AT
ATOM	5861	O	HOH	262	15.919	8.802	51.909	1.00	37.27	AT
ATOM	5862	O	HOH	263	60.591	34.941	-9.345	1.00	36.16	AT
ATOM	5863	O	HOH	264	10.541	36.936	29.724	1.00	38.71	AT
ATOM	5864	O	HOH	265	31.514	44.281	21.202	1.00	36.97	AT
ATOM	5865	O	HOH	266	9.564	36.687	51.380	1.00	38.68	AT
ATOM	5866	O	HOH	267	79.927	33.538	17.348	1.00	38.09	AT
ATOM	5867	O	HOH	268	52.604	28.637	11.241	1.00	38.37	AT
ATOM	5868	O	HOH	269	4.383	30.021	19.676	1.00	37.95	AT
ATOM	5869	O	HOH	270	39.831	37.961	44.275	1.00	39.26	AT
ATOM	5870	O	HOH	271	76.908	49.901	-8.433	1.00	40.20	AT

FIG. 1A-103

ATOM	5871	O	HOH	272	18.828	14.845	36.392	1.00	40.61	AT
ATOM	5872	O	HOH	273	77.377	18.239	12.575	1.00	39.42	AT
ATOM	5873	O	HOH	274	51.042	29.821	13.536	1.00	39.59	AT
ATOM	5874	O	HOH	275	64.107	14.629	14.266	1.00	39.71	AT
ATOM	5875	O	HOH	276	58.267	58.162	-7.799	1.00	39.43	AT
ATOM	5876	O	HOH	277	40.740	40.966	31.483	1.00	40.51	AT
ATOM	5877	O	HOH	278	15.055	10.589	55.645	1.00	39.15	AT
ATOM	5878	O	HOH	279	19.789	34.347	51.860	1.00	40.37	AT
ATOM	5879	O	HOH	280	11.976	38.727	31.710	1.00	37.91	AT
ATOM	5880	O	HOH	281	31.389	28.117	42.824	1.00	40.91	AT
ATOM	5881	O	HOH	282	70.878	25.270	-4.197	1.00	43.53	AT
ATOM	5882	O	HOH	283	75.431	41.776	4.726	1.00	40.67	AT
ATOM	5883	O	HOH	284	62.312	53.358	28.086	1.00	40.98	AT
ATOM	5884	O	HOH	285	62.124	59.105	9.640	1.00	39.55	AT
ATOM	5885	O	HOH	286	40.707	28.142	23.532	1.00	44.54	AT
ATOM	5886	O	HOH	287	33.311	41.660	3.153	1.00	41.98	AT
ATOM	5887	O	HOH	288	38.680	48.495	32.258	1.00	44.14	AT
ATOM	5888	O	HOH	289	32.712	38.251	44.880	1.00	40.32	AT
ATOM	5889	O	HOH	290	12.709	24.006	64.828	1.00	40.21	AT
ATOM	5890	O	HOH	291	48.861	28.304	14.453	1.00	42.61	AT
ATOM	5891	O	HOH	292	79.466	20.245	8.333	1.00	40.49	AT
ATOM	5892	O	HOH	293	50.553	45.041	-0.292	1.00	42.19	AT
ATOM	5893	O	HOH	294	42.897	26.326	5.722	1.00	41.10	AT
ATOM	5894	O	HOH	295	40.124	38.889	3.911	1.00	42.97	AT
ATOM	5895	O	HOH	296	-9.725	26.259	40.147	1.00	43.57	AT
ATOM	5896	O	HOH	297	24.463	39.296	47.536	1.00	39.76	AT
ATOM	5897	O	HOH	298	59.389	43.519	-22.049	1.00	45.90	AT
ATOM	5898	O	HOH	299	58.697	26.078	-8.432	1.00	42.64	AT
ATOM	5899	O	HOH	300	59.168	23.233	-8.586	1.00	43.13	AT
ATOM	5900	O	HOH	301	33.173	10.853	42.976	1.00	43.47	AT
ATOM	5901	O	HOH	302	38.135	51.041	21.685	1.00	40.23	AT
ATOM	5902	O	HOH	303	64.003	32.204	20.781	1.00	39.51	AT
ATOM	5903	O	HOH	304	18.175	36.881	18.239	1.00	42.51	AT
ATOM	5904	O	HOH	305	35.383	27.547	41.161	1.00	46.62	AT
ATOM	5905	O	HOH	306	-1.325	41.441	28.735	1.00	43.36	AT
ATOM	5906	O	HOH	307	18.409	47.629	30.260	1.00	46.92	AT
ATOM	5907	O	HOH	308	-0.365	41.851	31.323	1.00	43.06	AT
ATOM	5908	O	HOH	309	31.846	13.357	43.817	1.00	49.55	AT
ATOM	5909	O	HOH	310	51.910	47.621	-1.442	1.00	43.27	AT
ATOM	5910	O	HOH	311	29.562	44.918	17.110	1.00	52.42	AT
ATOM	5911	O	HOH	312	30.495	43.251	13.422	1.00	45.47	AT
ATOM	5912	O	HOH	313	11.474	10.744	42.423	1.00	51.55	AT
ATOM	5913	O	HOH	314	14.240	10.741	46.442	1.00	43.12	AT
ATOM	5914	O	HOH	315	52.861	58.416	6.793	1.00	44.59	AT
ATOM	5915	O	HOH	316	28.512	44.265	22.711	1.00	45.20	AT
ATOM	5916	O	HOH	317	72.643	46.339	-17.391	1.00	46.70	AT
ATOM	5917	O	HOH	318	31.387	46.123	19.248	1.00	43.61	AT
ATOM	5918	O	HOH	319	78.102	45.702	-8.575	1.00	48.47	AT
ATOM	5919	O	HOH	320	53.628	13.801	9.167	1.00	49.46	AT
ATOM	5920	O	HOH	321	65.846	41.632	-7.173	1.00	44.55	AT
ATOM	5921	O	HOH	322	41.074	48.539	27.174	1.00	50.50	AT
ATOM	5922	O	HOH	323	30.457	41.713	20.027	1.00	47.21	AT
ATOM	5923	O	HOH	324	23.888	42.661	19.783	1.00	49.37	AT
ATOM	5924	O	HOH	325	46.169	56.278	15.804	1.00	51.43	AT
ATOM	5925	O	HOH	326	64.632	36.604	-9.385	1.00	48.35	AT
ATOM	5926	O	HOH	327	50.410	48.704	-3.435	1.00	48.93	AT
ATOM	5927	O	HOH	328	17.266	4.657	48.965	1.00	55.69	AT

FIG. 1A-104

ATOM	5928	O	HOH	329	15.343	49.959	36.887	1.00 53.08	AT
ATOM	5929	O	HOH	330	77.778	42.870	3.924	1.00 55.32	AT
ATOM	5930	O	HOH	331	68.103	40.973	-5.266	1.00 57.57	AT
ATOM	5931	O	HOH	332	21.493	20.139	67.130	1.00 33.16	AT
ATOM	5932	O	HOH	333	81.269	24.355	14.982	1.00 33.69	AT
ATOM	5933	O	HOH	334	-5.903	30.538	26.686	1.00 40.35	AT
ATOM	5934	O	HOH	335	80.030	32.515	-0.810	1.00 39.92	AT
ATOM	5935	O	HOH	336	-7.205	27.318	42.127	1.00 37.50	AT
ATOM	5936	O	HOH	337	0.251	35.076	40.556	1.00 41.65	AT
ATOM	5937	O	HOH	338	67.263	58.975	-10.701	1.00 34.16	AT
ATOM	5938	O	HOH	339	78.930	41.885	0.871	1.00 36.88	AT
ATOM	5939	O	HOH	340	81.589	22.534	9.006	1.00 32.20	AT
ATOM	5940	O	HOH	341	-4.841	30.109	35.827	1.00 39.55	AT
ATOM	5941	O	HOH	342	24.216	28.828	53.120	1.00 48.54	AT
ATOM	5942	O	HOH	343	58.172	44.547	-15.457	1.00 37.88	AT
ATOM	5943	O	HOH	344	72.009	58.325	-12.680	1.00 44.56	AT
ATOM	5944	O	HOH	345	70.243	44.553	-16.741	1.00 37.48	AT
ATOM	5945	O	HOH	346	63.182	47.822	-22.683	1.00 47.83	AT
ATOM	5946	O	HOH	347	59.201	59.513	-12.511	1.00 48.60	AT
ATOM	5947	O	HOH	348	73.024	32.150	-1.717	1.00 35.73	AT
ATOM	5948	O	HOH	349	36.241	17.553	55.406	1.00 43.52	AT
ATOM	5949	O	HOH	351	14.204	56.480	33.327	1.00 44.23	AT
ATOM	5950	O	HOH	352	81.607	27.771	10.204	1.00 46.37	AT
ATOM	5951	O	HOH	353	72.230	29.150	-2.863	1.00 44.64	AT
ATOM	5952	O	HOH	354	63.965	35.398	-19.062	1.00 40.75	AT
ATOM	5953	O	HOH	355	83.662	27.262	2.560	1.00 52.07	AT
ATOM	5954	O	HOH	356	54.821	57.411	-7.143	1.00 47.42	AT
ATOM	5955	O	HOH	357	75.827	24.345	-2.592	1.00 38.53	AT
ATOM	5956	O	HOH	358	-3.100	29.989	33.712	1.00 35.26	AT
ATOM	5957	O	HOH	359	76.580	32.031	17.038	1.00 45.16	AT
ATOM	5958	O	HOH	360	61.004	63.374	-0.717	1.00 51.75	AT
ATOM	5959	O	HOH	361	57.555	42.914	-17.566	1.00 37.15	AT
ATOM	5960	O	HOH	362	46.758	41.005	-9.571	1.00 49.08	AT
ATOM	5961	O	HOH	363	65.046	41.921	10.931	1.00 43.73	AT
ATOM	5962	O	HOH	364	60.495	37.070	-20.999	1.00 39.43	AT
ATOM	5963	O	HOH	365	24.639	46.742	50.064	1.00 49.54	AT
ATOM	5964	O	HOH	366	65.360	59.537	-12.244	1.00 42.08	AT
ATOM	5965	O	HOH	367	81.253	38.379	6.191	1.00 44.60	AT
ATOM	5966	O	HOH	368	20.278	58.789	32.999	1.00 51.96	AT
ATOM	5967	O	HOH	369	35.754	25.608	43.846	1.00 41.69	AT
ATOM	5968	O	HOH	370	58.812	30.456	20.182	1.00 47.60	AT
ATOM	5969	O	HOH	371	62.070	60.522	-12.130	1.00 38.66	AT
ATOM	5970	O	HOH	372	28.704	57.271	37.789	1.00 53.91	AT
ATOM	5971	O	HOH	373	16.768	31.252	63.214	1.00 43.22	AT
ATOM	5972	O	HOH	374	17.431	24.978	67.168	1.00 45.45	AT
ATOM	5973	O	HOH	375	51.911	28.483	-4.087	1.00 57.67	AT
ATOM	5974	O	HOH	376	61.859	13.653	15.354	1.00 48.16	AT
ATOM	5975	O	HOH	377	60.309	37.228	-7.635	1.00 40.72	AT
ATOM	5976	O	HOH	378	76.341	49.000	11.927	1.00 51.08	AT
ATOM	5977	O	HOH	379	26.911	4.583	49.436	1.00 50.11	AT
ATOM	5978	O	HOH	380	60.796	28.003	14.825	1.00 41.08	AT
ATOM	5979	O	HOH	381	64.912	34.210	-13.805	1.00 54.13	AT
ATOM	5980	O	HOH	382	24.406	25.422	35.245	1.00 46.00	AT
ATOM	5981	O	HOH	383	27.206	10.460	58.142	1.00 48.67	AT
ATOM	5982	O	HOH	384	69.870	64.847	0.287	1.00 51.86	AT
ATOM	5983	O	HOH	385	13.388	53.599	30.313	1.00 53.21	AT
ATOM	5984	O	HOH	386	65.207	44.282	-23.032	1.00 44.87	AT

FIG. 1A-105

ATOM	5985	O	HOH	387	23.812	43.965	31.871	1.00	51.01	AT
ATOM	5986	O	HOH	388	27.925	56.723	25.402	1.00	50.91	AT
ATOM	5987	O	HOH	389	22.429	53.122	37.372	1.00	40.24	AT
ATOM	5988	O	HOH	390	20.340	37.818	64.894	1.00	43.91	AT
ATOM	5989	O	HOH	391	3.772	17.279	18.046	1.00	55.83	AT
ATOM	5990	O	HOH	392	61.560	29.447	-8.011	1.00	48.85	AT
ATOM	5991	O	HOH	393	40.737	49.676	12.185	1.00	48.28	AT
ATOM	5992	O	HOH	394	47.566	44.388	26.446	1.00	47.81	AT
ATOM	5993	O	HOH	395	62.091	37.019	27.629	1.00	53.63	AT
ATOM	5994	O	HOH	396	45.170	49.972	14.734	1.00	52.56	AT
ATOM	5995	O	HOH	397	25.713	56.378	37.487	1.00	46.30	AT
ATOM	5996	O	HOH	398	19.430	54.171	39.827	1.00	43.81	AT
ATOM	5997	O	HOH	399	25.461	13.937	28.867	1.00	46.75	AT
ATOM	5998	O	HOH	400	65.078	42.400	27.343	1.00	58.24	AT
ATOM	5999	O	HOH	401	15.750	35.665	16.140	1.00	49.43	AT
ATOM	6000	O	HOH	402	30.823	49.012	9.778	1.00	49.25	AT
ATOM	6001	O	HOH	403	63.642	30.868	-6.737	1.00	63.10	AT
ATOM	6002	O	HOH	404	-5.102	30.693	29.722	1.00	44.38	AT
ATOM	6003	O	HOH	405	5.998	28.463	48.599	1.00	45.41	AT
ATOM	6004	O	HOH	406	78.918	22.759	14.469	1.00	48.83	AT
ATOM	6005	O	HOH	407	67.800	14.615	-0.774	1.00	47.19	AT
ATOM	6006	O	HOH	408	-8.454	30.970	25.750	1.00	52.46	AT
ATOM	6007	O	HOH	409	39.982	27.102	31.435	1.00	51.86	AT
ATOM	6008	O	HOH	410	73.123	40.475	21.437	1.00	60.13	AT
ATOM	6009	O	HOH	411	60.888	14.040	1.887	1.00	46.41	AT
ATOM	6010	O	HOH	412	36.503	50.699	10.642	1.00	54.16	AT
ATOM	6011	O	HOH	413	59.362	62.211	-6.530	1.00	49.09	AT
ATOM	6012	O	HOH	414	28.103	13.240	52.474	1.00	47.88	AT
ATOM	6013	O	HOH	415	32.010	21.506	60.871	1.00	51.04	AT
ATOM	6014	O	HOH	416	35.534	13.760	51.867	1.00	48.76	AT
ATOM	6015	O	HOH	417	40.198	51.587	23.313	1.00	47.59	AT
ATOM	6016	O	HOH	418	32.582	27.322	18.391	1.00	59.17	AT
ATOM	6017	O	HOH	419	70.979	43.580	-23.023	1.00	62.55	AT
ATOM	6018	O	HOH	420	72.711	52.348	-21.252	1.00	55.53	AT
ATOM	6019	O	HOH	421	51.501	60.903	2.181	1.00	56.42	AT
ATOM	6020	O	HOH	423	53.460	21.733	-0.240	1.00	63.43	AT
ATOM	6021	O	HOH	424	55.865	19.944	-0.930	1.00	45.43	AT
ATOM	6022	O	HOH	425	11.457	18.171	63.981	1.00	40.96	AT
ATOM	6023	O	HOH	426	29.667	28.514	52.029	1.00	40.86	AT
ATOM	6024	O	HOH	427	21.382	43.057	31.379	1.00	37.88	AT
ATOM	6025	O	HOH	428	72.431	56.442	-14.816	1.00	38.78	AT
ATOM	6026	O	HOH	429	13.645	35.387	57.232	1.00	45.75	AT
ATOM	6027	O	HOH	430	47.325	44.655	9.515	1.00	52.79	AT
ATOM	6028	O	HOH	431	12.413	9.161	45.090	1.00	53.71	AT
ATOM	6029	O	HOH	432	69.847	39.107	-2.341	1.00	47.46	AT
ATOM	6030	O	HOH	433	40.580	34.476	3.546	1.00	42.74	AT
ATOM	6031	O	HOH	434	68.590	27.199	-5.061	1.00	50.14	AT
ATOM	6032	O	HOH	435	81.709	33.738	20.448	1.00	51.49	AT
ATOM	6033	O	HOH	436	21.276	6.862	53.221	1.00	43.81	AT
ATOM	6034	O	HOH	437	63.959	28.541	24.084	1.00	48.89	AT
ATOM	6035	O	HOH	438	44.540	42.464	26.796	1.00	45.92	AT
ATOM	6036	O	HOH	439	26.430	12.510	54.374	1.00	41.22	AT
ATOM	6037	O	HOH	440	13.505	42.803	49.080	1.00	49.02	AT
ATOM	6038	O	HOH	441	61.236	27.483	-9.781	1.00	53.99	AT
ATOM	6039	O	HOH	442	48.452	32.235	26.577	1.00	39.84	AT
ATOM	6040	O	HOH	443	-6.734	17.777	28.953	1.00	43.66	AT
ATOM	6041	O	HOH	444	68.689	11.054	1.803	1.00	54.43	AT

FIG. 1A-106

ATOM	6042	O	HOH	445	64.733	8.182	7.092	1.00	51.11	AT
ATOM	6043	O	HOH	446	47.452	47.307	25.789	1.00	50.83	AT
ATOM	6044	O	HOH	447	-5.597	17.191	22.022	1.00	62.54	AT
ATOM	6045	O	HOH	448	34.703	54.274	40.793	1.00	43.46	AT
ATOM	6046	O	HOH	449	7.584	42.423	41.797	1.00	50.29	AT
ATOM	6047	O	HOH	450	68.745	9.611	12.516	1.00	44.55	AT
ATOM	6048	O	HOH	451	10.345	30.448	14.624	1.00	52.09	AT
ATOM	6049	O	HOH	452	28.739	24.654	67.367	1.00	43.81	AT
ATOM	6050	O	HOH	453	59.859	15.451	-0.538	1.00	50.23	AT
ATOM	6051	O	HOH	454	9.715	22.615	40.260	1.00	55.68	AT
ATOM	6052	O	HOH	455	8.408	33.305	58.554	1.00	48.77	AT
ATOM	6053	O	HOH	456	82.808	20.346	7.688	1.00	64.19	AT
ATOM	6054	O	HOH	457	20.676	9.525	40.046	1.00	47.64	AT
ATOM	6055	O	HOH	458	12.300	21.911	45.521	1.00	55.95	AT
ATOM	6056	O	HOH	459	12.849	37.059	54.956	1.00	47.15	AT
ATOM	6057	O	HOH	460	18.947	37.315	56.296	1.00	55.87	AT
ATOM	6058	O	HOH	461	42.279	43.046	32.215	1.00	55.34	AT
ATOM	6059	O	HOH	462	58.113	60.078	-9.775	1.00	41.21	AT
ATOM	6060	O	HOH	463	-4.882	24.186	43.569	1.00	49.34	AT
ATOM	6061	O	HOH	464	2.275	30.894	44.638	1.00	49.59	AT
ATOM	6062	O	HOH	465	11.908	42.581	46.538	1.00	54.17	AT
ATOM	6063	O	HOH	466	25.196	30.973	68.678	1.00	54.36	AT
ATOM	6064	O	HOH	467	55.729	18.620	-3.586	1.00	51.13	AT
ATOM	6065	O	HOH	468	12.016	5.491	40.550	1.00	54.15	AT
ATOM	6066	O	HOH	469	56.711	29.214	27.406	1.00	63.41	AT
ATOM	6067	O	HOH	470	56.150	18.575	3.127	1.00	57.43	AT
ATOM	6068	O	HOH	471	18.186	11.646	26.302	1.00	54.34	AT
ATOM	6069	S1	DTT	1	74.181	38.187	-0.498	1.00	67.01	TT1
ATOM	6070	C1	DTT	1	72.670	38.130	-1.524	1.00	67.92	TT1
ATOM	6071	C2	DTT	1	72.656	36.968	-2.590	1.00	68.22	TT1
ATOM	6072	O2	DTT	1	71.393	37.023	-3.311	1.00	68.98	TT1
ATOM	6073	C3	DTT	1	73.769	37.036	-3.768	1.00	67.93	TT1
ATOM	6074	O3	DTT	1	73.674	35.873	-4.701	1.00	67.85	TT1
ATOM	6075	C4	DTT	1	75.213	37.003	-3.287	1.00	67.57	TT1
ATOM	6076	S4	DTT	1	75.541	38.418	-2.099	1.00	67.52	TT1
ATOM	6077	S1	DTT	2	54.935	53.026	7.820	1.00	53.56	TT2
ATOM	6078	C1	DTT	2	53.759	51.637	7.760	1.00	53.84	TT2
ATOM	6079	C2	DTT	2	52.738	51.710	6.562	1.00	54.90	TT2
ATOM	6080	O2	DTT	2	51.885	50.534	6.613	1.00	56.10	TT2
ATOM	6081	C3	DTT	2	51.681	52.940	6.568	1.00	54.93	TT2
ATOM	6082	O3	DTT	2	50.780	52.918	5.376	1.00	55.43	TT2
ATOM	6083	C4	DTT	2	52.313	54.325	6.524	1.00	54.51	TT2
ATOM	6084	S4	DTT	2	53.485	54.549	7.971	1.00	54.25	TT2
ATOM	6085	S1	DTT	3	9.841	19.197	19.765	1.00	46.94	TT3
ATOM	6086	C1	DTT	3	8.080	19.681	19.855	1.00	44.23	TT3
ATOM	6087	C2	DTT	3	7.123	18.477	20.203	1.00	45.91	TT3
ATOM	6088	O2	DTT	3	5.758	18.968	20.283	1.00	45.68	TT3
ATOM	6089	C3	DTT	3	7.023	17.285	19.113	1.00	46.42	TT3
ATOM	6090	O3	DTT	3	6.110	16.195	19.567	1.00	49.11	TT3
ATOM	6091	C4	DTT	3	8.337	16.568	18.812	1.00	45.21	TT3
ATOM	6092	S4	DTT	3	9.629	17.785	18.211	1.00	44.44	TT3
ATOM	6093	S1	DTT	4	19.785	34.825	23.721	1.00	49.21	TT4
ATOM	6094	C1	DTT	4	19.784	36.095	25.038	1.00	49.59	TT4
ATOM	6095	C2	DTT	4	18.556	37.084	24.993	1.00	51.01	TT4
ATOM	6096	O2	DTT	4	18.673	38.019	26.105	1.00	52.92	TT4
ATOM	6097	C3	DTT	4	18.440	38.051	23.699	1.00	50.89	TT4
ATOM	6098	O3	DTT	4	17.234	38.926	23.759	1.00	51.66	TT4

FIG. 1A-107


```
ATOM   6099  C4  DTT     4      18.302  37.325  22.365  1.00 50.07      TT4
ATOM   6100  S4  DTT     4      19.750  36.164  22.087  1.00 49.50      TT4
ATOM   6101  S1  DTT     5      13.883  15.968  40.130  1.00 53.89      TT5
ATOM   6102  C1  DTT     5      12.694  17.323  39.827  1.00 54.86      TT5
ATOM   6103  C2  DTT     5      11.608  17.502  40.955  1.00 55.83      TT5
ATOM   6104  O2  DTT     5      10.754  18.625  40.590  1.00 57.35      TT5
ATOM   6105  C3  DTT     5      10.561  16.283  41.172  1.00 55.92      TT5
ATOM   6106  O3  DTT     5       9.597  16.559  42.278  1.00 56.47      TT5
ATOM   6107  C4  DTT     5      11.194  14.953  41.564  1.00 55.56      TT5
ATOM   6108  S4  DTT     5      12.443  14.418  40.274  1.00 55.31      TT5
ATOM   6109  C1  GOL     6      25.840  30.485  23.369  1.00 60.12      OL1
ATOM   6110  O1  GOL     6      24.418  30.344  23.510  1.00 58.37      OL1
ATOM   6111  C2  GOL     6      26.254  30.565  21.841  1.00 60.62      OL1
ATOM   6112  O2  GOL     6      26.921  31.825  21.610  1.00 61.53      OL1
ATOM   6113  C3  GOL     6      25.019  30.470  20.890  1.00 60.48      OL1
ATOM   6114  O3  GOL     6      25.353  30.640  19.507  1.00 60.02      OL1
ATOM   6115  C1  GOL     7      79.028  22.813  10.783  1.00 59.60      OL2
ATOM   6116  O1  GOL     7      78.201  22.510  11.912  1.00 61.71      OL2
ATOM   6117  C2  GOL     7      79.615  24.278  10.893  1.00 59.54      OL2
ATOM   6118  O2  GOL     7      81.057  24.201  10.902  1.00 59.72      OL2
ATOM   6119  C3  GOL     7      79.147  25.010  12.189  1.00 58.44      OL2
ATOM   6120  O3  GOL     7      79.958  26.145  12.514  1.00 56.91      OL2
ATOM   6121 NA+1 NA1    1      63.339  31.566  -2.590  1.00 26.24      ONS
ATOM   6122 NA+1 NA1    2      65.507  33.113  17.476  1.00 24.78      ONS
ATOM   6123 NA+1 NA1    3      52.138  43.339  -0.467  1.00 31.32      ONS
ATOM   6124 NA+1 NA1    4      11.564  27.003  46.250  1.00 28.57      ONS
ATOM   6125 NA+1 NA1    5      22.858  38.903  45.868  1.00 35.79      ONS
ATOM   6126 NA+1 NA1    6      12.049  37.399  33.606  1.00 30.07      ONS
ATOM   6127 NA+1 NA1    7      52.399  30.404   9.576  1.00 28.65      ONS
ATOM   6128 NA+1 NA1    8      61.322  58.273 -12.969  1.00 38.12      ONS
ATOM   6129 CL-1 CL1    9      74.315  48.004  -8.768  1.00 36.69      ONS
ATOM   6130 CL-1 CL1   10      10.448  28.591  48.519  1.00 26.89      ONS
ATOM   6131 CL-1 CL1   11      49.897  29.847   8.163  1.00 28.28      ONS
ATOM   6132 CL-1 CL1   12      68.370  32.685  17.763  1.00 30.08      ONS
ATOM   6133 CL-1 CL1   13      21.352  41.348  46.322  1.00 33.00      ONS
ATOM   6134 CL-1 CL1   14      21.514  34.817  28.080  1.00 20.85      ONS
ATOM   6135 CL-1 CL1   15      70.235  40.020   0.588  1.00 21.12      ONS
ATOM   6136 CL-1 CL1   16      55.303  48.583   9.136  1.00 22.36      ONS
ATOM   6137 CL-1 CL1   17      61.816  29.359  -3.630  1.00 27.78      ONS
ATOM   6138 CL-1 CL1   18      66.265  35.653  18.338  1.00 26.36      ONS
ATOM   6139 CL-1 CL1   19       9.405  38.244  34.766  1.00 27.56      ONS
ATOM   6140 CL-1 CL1   20      56.075  30.580  -5.205  1.00 30.76      ONS
ATOM   6141 CL-1 CL1   21      51.184  42.277  -2.989  1.00 29.31      ONS
ATOM   6142 CL-1 CL1   22       8.488  34.106  46.950  1.00 31.69      ONS
ATOM   6143 CL-1 CL1   23      26.255  30.563  26.909  1.00 29.29      ONS
ATOM   6144 CL-1 CL1   24      14.532  19.865  38.018  1.00 22.44      ONS
ATOM   6145 CL-1 CL1   25      38.459  48.451  29.075  1.00 41.86      ONS
ATOM   6146 CL-1 CL1   26      48.969  36.502  -2.659  1.00 32.79      ONS
ATOM   6147 CL-1 CL1   27      19.241  17.587  34.034  1.00 29.08      ONS
END
```

FIG. 2

		Atom Type	Res.		X	Y	Z	OCC	B	MOL
ATOM	1	C	GLY	1	3.531	2.676	31.918	1.00	23.54	ACPS
ATOM	2	O	GLY	1	2.877	3.712	32.042	1.00	24.07	ACPS
ATOM	3	N	GLY	1	3.058	2.705	29.459	1.00	25.97	ACPS
ATOM	4	CA	GLY	1	3.503	1.884	30.623	1.00	24.19	ACPS
ATOM	5	N	ILE	2	4.299	2.191	32.884	1.00	21.88	ACPS
ATOM	6	CA	ILE	2	4.396	2.857	34.180	1.00	20.22	ACPS
ATOM	7	CB	ILE	2	4.119	1.857	35.329	1.00	19.41	ACPS
ATOM	8	CG2	ILE	2	4.474	2.485	36.679	1.00	18.46	ACPS
ATOM	9	CG1	ILE	2	2.647	1.429	35.289	1.00	19.13	ACPS

FIG. 2A-1


```
ATOM     10  CD1 ILE     2       2.303   0.294  36.250  1.00 20.56      ACPS
ATOM     11  C   ILE     2       5.769   3.490  34.376  1.00 19.58      ACPS
ATOM     12  O   ILE     2       6.798   2.827  34.223  1.00 19.75      ACPS
ATOM     13  N   TYR     3       5.779   4.780  34.704  1.00 18.83      ACPS
ATOM     14  CA  TYR     3       7.024   5.493  34.942  1.00 18.94      ACPS
ATOM     15  CB  TYR     3       6.814   7.004  34.809  1.00 21.16      ACPS
ATOM     16  CG  TYR     3       8.059   7.808  35.103  1.00 23.30      ACPS
ATOM     17  CD1 TYR     3       9.164   7.761  34.246  1.00 24.81      ACPS
ATOM     18  CE1 TYR     3      10.326   8.486  34.525  1.00 25.94      ACPS
ATOM     19  CD2 TYR     3       8.145   8.601  36.246  1.00 24.18      ACPS
ATOM     20  CE2 TYR     3       9.297   9.329  36.534  1.00 25.63      ACPS
ATOM     21  CZ  TYR     3      10.384   9.267  35.672  1.00 26.92      ACPS
ATOM     22  OH  TYR     3      11.524   9.974  35.970  1.00 28.98      ACPS
ATOM     23  C   TYR     3       7.555   5.165  36.340  1.00 17.87      ACPS
ATOM     24  O   TYR     3       8.757   4.968  36.525  1.00 18.51      ACPS
ATOM     25  N   GLY     4       6.657   5.107  37.325  1.00 16.17      ACPS
ATOM     26  CA  GLY     4       7.088   4.789  38.678  1.00 13.94      ACPS
ATOM     27  C   GLY     4       5.937   4.643  39.657  1.00 13.19      ACPS
ATOM     28  O   GLY     4       4.819   5.094  39.387  1.00 13.25      ACPS
ATOM     29  N   ILE     5       6.217   4.001  40.794  1.00 12.43      ACPS
ATOM     30  CA  ILE     5       5.209   3.822  41.841  1.00 11.10      ACPS
ATOM     31  CB  ILE     5       4.718   2.326  41.963  1.00 11.22      ACPS
ATOM     32  CG2 ILE     5       4.330   1.793  40.572  1.00 12.21      ACPS
ATOM     33  CG1 ILE     5       5.785   1.441  42.619  1.00 11.21      ACPS
ATOM     34  CD1 ILE     5       5.338  -0.010  42.831  1.00 12.31      ACPS
ATOM     35  C   ILE     5       5.793   4.294  43.175  1.00 10.72      ACPS
ATOM     36  O   ILE     5       7.013   4.358  43.346  1.00 11.21      ACPS
ATOM     37  N   GLY     6       4.910   4.644  44.108  1.00 10.20      ACPS
ATOM     38  CA  GLY     6       5.347   5.102  45.414  1.00  9.68      ACPS
ATOM     39  C   GLY     6       4.348   4.762  46.503  1.00 10.17      ACPS
ATOM     40  O   GLY     6       3.139   4.776  46.261  1.00  9.96      ACPS
ATOM     41  N   LEU     7       4.859   4.459  47.697  1.00  9.09      ACPS
ATOM     42  CA  LEU     7       4.024   4.109  48.852  1.00  9.72      ACPS
ATOM     43  CB  LEU     7       4.058   2.588  49.078  1.00 10.10      ACPS
ATOM     44  CG  LEU     7       3.308   2.001  50.285  1.00  9.72      ACPS
ATOM     45  CD1 LEU     7       1.814   2.059  50.037  1.00 12.07      ACPS
ATOM     46  CD2 LEU     7       3.741   0.552  50.503  1.00 10.42      ACPS
ATOM     47  C   LEU     7       4.530   4.804  50.121  1.00 10.28      ACPS
ATOM     48  O   LEU     7       5.739   4.936  50.319  1.00 10.25      ACPS
ATOM     49  N   ASP     8       3.610   5.255  50.976  1.00  9.98      ACPS
ATOM     50  CA  ASP     8       4.024   5.871  52.230  1.00  9.91      ACPS
ATOM     51  CB  ASP     8       4.323   7.365  52.045  1.00  9.85      ACPS
ATOM     52  CG  ASP     8       5.223   7.887  53.128  1.00 11.38      ACPS
ATOM     53  OD1 ASP     8       4.723   8.465  54.110  1.00 12.14      ACPS
ATOM     54  OD2 ASP     8       6.439   7.672  53.003  1.00 13.58      ACPS
ATOM     55  C   ASP     8       2.997   5.715  53.338  1.00  9.65      ACPS
ATOM     56  O   ASP     8       1.792   5.822  53.101  1.00 10.65      ACPS
ATOM     57  N   ILE     9       3.479   5.447  54.551  1.00  9.53      ACPS
ATOM     58  CA  ILE     9       2.598   5.334  55.721  1.00  9.56      ACPS
ATOM     59  CB  ILE     9       2.634   3.913  56.338  1.00  9.26      ACPS
ATOM     60  CG2 ILE     9       1.780   3.890  57.602  1.00 10.57      ACPS
ATOM     61  CG1 ILE     9       2.101   2.881  55.338  1.00  9.47      ACPS
ATOM     62  CD1 ILE     9       2.215   1.426  55.815  1.00 10.23      ACPS
ATOM     63  C   ILE     9       3.142   6.361  56.717  1.00  9.80      ACPS
ATOM     64  O   ILE     9       4.233   6.206  57.245  1.00  9.76      ACPS
ATOM     65  N   THR    10       2.375   7.423  56.941  1.00  9.46      ACPS
ATOM     66  CA  THR    10       2.768   8.527  57.819  1.00 10.38      ACPS
```

FIG. 2A-2

ATOM	67	CB	THR	10	2.428	9.871	57.089	1.00	10.26	ACPS
ATOM	68	OG1	THR	10	3.340	10.050	55.997	1.00	11.15	ACPS
ATOM	69	CG2	THR	10	2.527	11.081	58.021	1.00	11.35	ACPS
ATOM	70	C	THR	10	2.113	8.453	59.211	1.00	10.55	ACPS
ATOM	71	O	THR	10	0.936	8.111	59.336	1.00	10.38	ACPS
ATOM	72	N	GLU	11	2.897	8.773	60.246	1.00	10.75	ACPS
ATOM	73	CA	GLU	11	2.463	8.743	61.654	1.00	11.46	ACPS
ATOM	74	CB	GLU	11	3.708	8.583	62.544	1.00	11.49	ACPS
ATOM	75	CG	GLU	11	3.454	8.435	64.044	1.00	14.01	ACPS
ATOM	76	CD	GLU	11	3.151	7.005	64.449	1.00	16.01	ACPS
ATOM	77	OE1	GLU	11	3.674	6.084	63.791	1.00	17.38	ACPS
ATOM	78	OE2	GLU	11	2.417	6.807	65.435	1.00	18.05	ACPS
ATOM	79	C	GLU	11	1.697	10.012	62.065	1.00	11.12	ACPS
ATOM	80	O	GLU	11	2.255	11.106	62.037	1.00	11.41	ACPS
ATOM	81	N	LEU	12	0.430	9.865	62.447	1.00	11.46	ACPS
ATOM	82	CA	LEU	12	-0.383	11.026	62.848	1.00	12.27	ACPS
ATOM	83	CB	LEU	12	-1.785	10.582	63.305	1.00	12.68	ACPS
ATOM	84	CG	LEU	12	-2.751	10.062	62.234	1.00	13.69	ACPS
ATOM	85	CD1	LEU	12	-4.049	9.642	62.918	1.00	13.86	ACPS
ATOM	86	CD2	LEU	12	-3.039	11.140	61.183	1.00	14.80	ACPS
ATOM	87	C	LEU	12	0.265	11.839	63.963	1.00	12.67	ACPS
ATOM	88	O	LEU	12	0.270	13.066	63.915	1.00	12.56	ACPS
ATOM	89	N	LYS	13	0.826	11.158	64.958	1.00	13.19	ACPS
ATOM	90	CA	LYS	13	1.457	11.852	66.085	1.00	14.09	ACPS
ATOM	91	CB	LYS	13	1.878	10.851	67.165	1.00	15.99	ACPS
ATOM	92	CG	LYS	13	0.740	10.332	68.017	1.00	20.36	ACPS
ATOM	93	CD	LYS	13	1.290	9.557	69.197	1.00	23.47	ACPS
ATOM	94	CE	LYS	13	0.232	9.319	70.261	1.00	25.28	ACPS
ATOM	95	NZ	LYS	13	0.840	8.690	71.473	1.00	26.94	ACPS
ATOM	96	C	LYS	13	2.665	12.693	65.685	1.00	13.56	ACPS
ATOM	97	O	LYS	13	2.924	13.738	66.295	1.00	13.25	ACPS
ATOM	98	N	ARG	14	3.423	12.237	64.692	1.00	12.75	ACPS
ATOM	99	CA	ARG	14	4.579	13.009	64.233	1.00	13.17	ACPS
ATOM	100	CB	ARG	14	5.436	12.178	63.270	1.00	14.59	ACPS
ATOM	101	CG	ARG	14	6.598	12.936	62.661	1.00	17.45	ACPS
ATOM	102	CD	ARG	14	7.572	12.010	61.933	1.00	21.04	ACPS
ATOM	103	NE	ARG	14	8.623	12.770	61.254	1.00	23.74	ACPS
ATOM	104	CZ	ARG	14	8.689	12.966	59.939	1.00	25.19	ACPS
ATOM	105	NH1	ARG	14	7.768	12.450	59.134	1.00	25.79	ACPS
ATOM	106	NH2	ARG	14	9.671	13.701	59.425	1.00	15.80	ACPS
ATOM	107	C	ARG	14	4.100	14.296	63.547	1.00	13.10	ACPS
ATOM	108	O	ARG	14	4.636	15.377	63.798	1.00	13.21	ACPS
ATOM	109	N	ILE	15	3.099	14.181	62.678	1.00	11.73	ACPS
ATOM	110	CA	ILE	15	2.559	15.348	61.988	1.00	12.13	ACPS
ATOM	111	CB	ILE	15	1.468	14.924	60.965	1.00	12.16	ACPS
ATOM	112	CG2	ILE	15	0.822	16.150	60.320	1.00	13.81	ACPS
ATOM	113	CG1	ILE	15	2.095	14.050	59.875	1.00	13.13	ACPS
ATOM	114	CD1	ILE	15	3.191	14.736	59.050	1.00	15.37	ACPS
ATOM	115	C	ILE	15	1.981	16.356	62.996	1.00	12.43	ACPS
ATOM	116	O	ILE	15	2.165	17.571	62.845	1.00	13.17	ACPS
ATOM	117	N	ALA	16	1.292	15.859	64.019	1.00	12.31	ACPS
ATOM	118	CA	ALA	16	0.711	16.740	65.038	1.00	13.48	ACPS
ATOM	119	CB	ALA	16	-0.165	15.938	66.000	1.00	13.26	ACPS
ATOM	120	C	ALA	16	1.812	17.456	65.811	1.00	13.84	ACPS
ATOM	121	O	ALA	16	1.679	18.631	66.159	1.00	14.13	ACPS
ATOM	122	N	SER	17	2.902	16.752	66.089	1.00	13.89	ACPS
ATOM	123	CA	SER	17	4.013	17.356	66.809	1.00	14.78	ACPS

FIG. 2A-3

ATOM	124	CB	SER	17	5.041	16.291	67.199	1.00	14.52	ACPS
ATOM	125	OG	SER	17	6.151	16.878	67.861	1.00	15.33	ACPS
ATOM	126	C	SER	17	4.686	18.440	65.971	1.00	15.57	ACPS
ATOM	127	O	SER	17	4.981	19.528	66.478	1.00	16.23	ACPS
ATOM	128	N	MET	18	4.933	18.163	64.694	1.00	15.86	ACPS
ATOM	129	CA	MET	18	5.568	19.173	63.861	1.00	17.36	ACPS
ATOM	130	CB	MET	18	5.920	18.593	62.491	1.00	18.79	ACPS
ATOM	131	CG	MET	18	6.984	17.513	62.579	1.00	21.58	ACPS
ATOM	132	SD	MET	18	7.569	16.962	60.979	1.00	27.23	ACPS
ATOM	133	CE	MET	18	6.322	15.823	60.550	1.00	24.77	ACPS
ATOM	134	C	MET	18	4.679	20.408	63.724	1.00	18.05	ACPS
ATOM	135	O	MET	18	5.171	21.537	63.720	1.00	17.78	ACPS
ATOM	136	N	ALA	19	3.371	20.200	63.637	1.00	17.79	ACPS
ATOM	137	CA	ALA	19	2.439	21.320	63.519	1.00	19.33	ACPS
ATOM	138	CB	ALA	19	1.047	20.810	63.161	1.00	18.47	ACPS
ATOM	139	C	ALA	19	2.391	22.119	64.827	1.00	20.49	ACPS
ATOM	140	O	ALA	19	2.124	23.324	64.820	1.00	21.87	ACPS
ATOM	141	N	GLY	20	2.655	21.446	65.944	1.00	21.04	ACPS
ATOM	142	CA	GLY	20	2.635	22.112	67.234	1.00	22.79	ACPS
ATOM	143	C	GLY	20	3.916	22.879	67.506	1.00	24.03	ACPS
ATOM	144	O	GLY	20	3.920	23.834	68.283	1.00	25.21	ACPS
ATOM	145	N	ARG	21	5.007	22.463	66.875	1.00	24.92	ACPS
ATOM	146	CA	ARG	21	6.286	23.135	67.062	1.00	26.49	ACPS
ATOM	147	CB	ARG	21	7.420	22.117	67.058	1.00	27.00	ACPS
ATOM	148	CG	ARG	21	7.376	21.144	68.216	1.00	28.19	ACPS
ATOM	149	CD	ARG	21	8.764	20.607	68.471	1.00	29.42	ACPS
ATOM	150	NE	ARG	21	9.667	21.695	68.835	1.00	30.12	ACPS
ATOM	151	CZ	ARG	21	10.993	21.603	68.834	1.00	29.99	ACPS
ATOM	152	NH1	ARG	21	11.727	22.650	69.183	1.00	30.82	ACPS
ATOM	153	NH2	ARG	21	11.584	20.469	68.481	1.00	30.49	ACPS
ATOM	154	C	ARG	21	6.559	24.208	66.006	1.00	27.49	ACPS
ATOM	155	O	ARG	21	7.329	25.141	66.247	1.00	28.27	ACPS
ATOM	156	N	GLN	22	5.935	24.073	64.840	1.00	27.79	ACPS
ATOM	157	CA	GLN	22	6.103	25.039	63.757	1.00	28.18	ACPS
ATOM	158	CB	GLN	22	6.697	24.364	62.515	1.00	29.33	ACPS
ATOM	159	CG	GLN	22	8.186	24.075	62.625	1.00	30.67	ACPS
ATOM	160	CD	GLN	22	8.839	23.775	61.284	1.00	31.99	ACPS
ATOM	161	OE1	GLN	22	10.065	23.853	61.148	1.00	33.50	ACPS
ATOM	162	NE2	GLN	22	8.029	23.422	60.291	1.00	31.08	ACPS
ATOM	163	C	GLN	22	4.765	25.686	63.406	1.00	27.71	ACPS
ATOM	164	O	GLN	22	3.866	25.036	62.869	1.00	27.85	ACPS
ATOM	165	N	ALA	23	4.646	26.976	63.707	1.00	26.91	ACPS
ATOM	166	CA	ALA	23	3.420	27.721	63.453	1.00	25.59	ACPS
ATOM	167	CB	ALA	23	3.578	29.155	63.945	1.00	26.37	ACPS
ATOM	168	C	ALA	23	2.966	27.722	61.994	1.00	24.20	ACPS
ATOM	169	O	ALA	23	1.784	27.936	61.711	1.00	25.27	ACPS
ATOM	170	N	ARG	24	3.885	27.478	61.068	1.00	22.39	ACPS
ATOM	171	CA	ARG	24	3.519	27.481	59.655	1.00	20.64	ACPS
ATOM	172	CB	ARG	24	4.265	28.617	58.943	1.00	23.30	ACPS
ATOM	173	CG	ARG	24	4.063	29.987	59.612	1.00	26.19	ACPS
ATOM	174	CD	ARG	24	4.793	31.085	58.862	1.00	30.07	ACPS
ATOM	175	NE	ARG	24	4.710	32.403	59.493	1.00	32.13	ACPS
ATOM	176	CZ	ARG	24	5.594	32.879	60.363	1.00	32.86	ACPS
ATOM	177	NH1	ARG	24	6.644	32.150	60.720	1.00	33.10	ACPS
ATOM	178	NH2	ARG	24	5.435	34.097	60.867	1.00	34.22	ACPS
ATOM	179	C	ARG	24	3.784	26.144	58.956	1.00	19.11	ACPS
ATOM	180	O	ARG	24	3.982	26.094	57.744	1.00	17.80	ACPS

FIG. 2A-4

ATOM	181	N	PHE	25	3.765	25.057	59.720	1.00	16.89	ACPS
ATOM	182	CA	PHE	25	4.007	23.738	59.147	1.00	16.15	ACPS
ATOM	183	CB	PHE	25	3.958	22.664	60.246	1.00	16.22	ACPS
ATOM	184	CG	PHE	25	4.308	21.282	59.757	1.00	16.81	ACPS
ATOM	185	CD1	PHE	25	3.357	20.271	59.754	1.00	17.39	ACPS
ATOM	186	CD2	PHE	25	5.577	21.008	59.255	1.00	16.97	ACPS
ATOM	187	CE1	PHE	25	3.662	19.001	59.253	1.00	18.39	ACPS
ATOM	188	CE2	PHE	25	5.892	19.737	58.752	1.00	18.24	ACPS
ATOM	189	CZ	PHE	25	4.930	18.737	58.753	1.00	17.96	ACPS
ATOM	190	C	PHE	25	3.038	23.370	58.015	1.00	15.11	ACPS
ATOM	191	O	PHE	25	3.464	22.840	56.988	1.00	14.64	ACPS
ATOM	192	N	ALA	26	1.748	23.646	58.196	1.00	15.46	ACPS
ATOM	193	CA	ALA	26	0.762	23.332	57.162	1.00	15.40	ACPS
ATOM	194	CB	ALA	26	-0.658	23.670	57.642	1.00	16.24	ACPS
ATOM	195	C	ALA	26	1.075	24.093	55.881	1.00	15.52	ACPS
ATOM	196	O	ALA	26	0.941	23.551	54.787	1.00	14.18	ACPS
ATOM	197	N	GLU	27	1.512	25.345	56.011	1.00	14.73	ACPS
ATOM	198	CA	GLU	27	1.839	26.155	54.838	1.00	15.35	ACPS
ATOM	199	CB	GLU	27	2.041	27.619	55.236	1.00	16.37	ACPS
ATOM	200	CG	GLU	27	0.782	28.381	55.603	1.00	18.60	ACPS
ATOM	201	CD	GLU	27	0.176	27.956	56.927	1.00	19.31	ACPS
ATOM	202	OE1	GLU	27	0.899	27.430	57.796	1.00	19.16	ACPS
ATOM	203	OE2	GLU	27	-1.040	28.169	57.109	1.00	22.95	ACPS
ATOM	204	C	GLU	27	3.089	25.652	54.115	1.00	14.38	ACPS
ATOM	205	O	GLU	27	3.309	25.946	52.944	1.00	14.80	ACPS
ATOM	206	N	ARG	28	3.907	24.896	54.829	1.00	15.20	ACPS
ATOM	207	CA	ARG	28	5.119	24.330	54.268	1.00	16.00	ACPS
ATOM	208	CB	ARG	28	6.018	23.880	55.420	1.00	18.75	ACPS
ATOM	209	CG	ARG	28	7.335	23.289	55.015	1.00	22.72	ACPS
ATOM	210	CD	ARG	28	8.158	22.968	56.250	1.00	25.44	ACPS
ATOM	211	NE	ARG	28	9.461	22.432	55.890	1.00	28.04	ACPS
ATOM	212	CZ	ARG	28	10.382	22.070	56.775	1.00	28.40	ACPS
ATOM	213	NH1	ARG	28	11.542	21.594	56.356	1.00	29.55	ACPS
ATOM	214	NH2	ARG	28	10.135	22.184	58.074	1.00	28.44	ACPS
ATOM	215	C	ARG	28	4.768	23.129	53.380	1.00	15.03	ACPS
ATOM	216	O	ARG	28	5.345	22.925	52.311	1.00	15.61	ACPS
ATOM	217	N	ILE	29	3.792	22.350	53.824	1.00	14.41	ACPS
ATOM	218	CA	ILE	29	3.396	21.137	53.112	1.00	14.00	ACPS
ATOM	219	CB	ILE	29	2.883	20.066	54.121	1.00	13.17	ACPS
ATOM	220	CG2	ILE	29	2.586	18.765	53.401	1.00	13.59	ACPS
ATOM	221	CG1	ILE	29	3.900	19.834	55.245	1.00	13.14	ACPS
ATOM	222	CD1	ILE	29	5.307	19.516	54.785	1.00	12.95	ACPS
ATOM	223	C	ILE	29	2.313	21.299	52.034	1.00	13.32	ACPS
ATOM	224	O	ILE	29	2.370	20.650	50.993	1.00	13.97	ACPS
ATOM	225	N	LEU	30	1.350	22.181	52.275	1.00	12.58	ACPS
ATOM	226	CA	LEU	30	0.211	22.337	51.369	1.00	12.60	ACPS
ATOM	227	CB	LEU	30	-1.073	22.390	52.207	1.00	12.43	ACPS
ATOM	228	CG	LEU	30	-1.309	21.263	53.220	1.00	12.14	ACPS
ATOM	229	CD1	LEU	30	-2.536	21.595	54.057	1.00	13.80	ACPS
ATOM	230	CD2	LEU	30	-1.496	19.932	52.491	1.00	12.77	ACPS
ATOM	231	C	LEU	30	0.227	23.540	50.432	1.00	12.66	ACPS
ATOM	232	O	LEU	30	0.732	24.605	50.785	1.00	14.05	ACPS
ATOM	233	N	THR	31	-0.342	23.359	49.242	1.00	13.04	ACPS
ATOM	234	CA	THR	31	-0.456	24.450	48.265	1.00	13.14	ACPS
ATOM	235	CB	THR	31	-0.746	23.921	46.859	1.00	13.54	ACPS
ATOM	236	OG1	THR	31	-2.018	23.262	46.854	1.00	13.92	ACPS
ATOM	237	CG2	THR	31	0.313	22.937	46.429	1.00	14.69	ACPS

FIG. 2A-5

ATOM	238	C	THR	31	-1.641	25.328	48.690	1.00 13.91	ACPS
ATOM	239	O	THR	31	-2.374	24.980	49.617	1.00 13.14	ACPS
ATOM	240	N	ARG	32	-1.836	26.455	48.014	1.00 15.34	ACPS
ATOM	241	CA	ARG	32	-2.947	27.338	48.367	1.00 15.55	ACPS
ATOM	242	CB	ARG	32	-2.912	28.615	47.517	1.00 16.36	ACPS
ATOM	243	CG	ARG	32	-1.630	29.403	47.682	1.00 18.69	ACPS
ATOM	244	CD	ARG	32	-1.794	30.834	47.191	1.00 20.77	ACPS
ATOM	245	NE	ARG	32	-2.750	31.590	48.000	1.00 22.37	ACPS
ATOM	246	CZ	ARG	32	-3.938	32.003	47.569	1.00 23.12	ACPS
ATOM	247	NH1	ARG	32	-4.326	31.738	46.330	1.00 23.58	ACPS
ATOM	248	NH2	ARG	32	-4.738	32.686	48.380	1.00 22.27	ACPS
ATOM	249	C	ARG	32	-4.296	26.646	48.205	1.00 15.92	ACPS
ATOM	250	O	ARG	32	-5.166	26.781	49.054	1.00 16.02	ACPS
ATOM	251	N	SER	33	-4.467	25.908	47.114	1.00 16.47	ACPS
ATOM	252	CA	SER	33	-5.717	25.183	46.863	1.00 16.46	ACPS
ATOM	253	CB	SER	33	-5.638	24.465	45.513	1.00 17.75	ACPS
ATOM	254	OG	SER	33	-6.833	23.772	45.224	1.00 24.08	ACPS
ATOM	255	C	SER	33	-5.981	24.154	47.967	1.00 16.53	ACPS
ATOM	256	O	SER	33	-7.115	23.963	48.404	1.00 16.86	ACPS
ATOM	257	N	GLU	34	-4.926	23.484	48.413	1.00 15.70	ACPS
ATOM	258	CA	GLU	34	-5.058	22.480	49.458	1.00 15.77	ACPS
ATOM	259	CB	GLU	34	-3.753	21.677	49.573	1.00 14.72	ACPS
ATOM	260	CG	GLU	34	-3.578	20.659	48.459	1.00 15.35	ACPS
ATOM	261	CD	GLU	34	-2.174	20.079	48.369	1.00 13.75	ACPS
ATOM	262	OE1	GLU	34	-2.023	19.029	47.719	1.00 13.81	ACPS
ATOM	263	OE2	GLU	34	-1.215	20.669	48.916	1.00 13.16	ACPS
ATOM	264	C	GLU	34	-5.397	23.134	50.789	1.00 15.99	ACPS
ATOM	265	O	GLU	34	-6.206	22.621	51.563	1.00 17.16	ACPS
ATOM	266	N	LEU	35	-4.781	24.285	51.050	1.00 16.62	ACPS
ATOM	267	CA	LEU	35	-5.025	25.008	52.285	1.00 17.38	ACPS
ATOM	268	CB	LEU	35	-4.064	26.199	52.401	1.00 17.16	ACPS
ATOM	269	CG	LEU	35	-2.614	25.863	52.761	1.00 17.73	ACPS
ATOM	270	CD1	LEU	35	-1.722	27.078	52.532	1.00 17.25	ACPS
ATOM	271	CD2	LEU	35	-2.547	25.405	54.212	1.00 17.05	ACPS
ATOM	272	C	LEU	35	-6.462	25.499	52.380	1.00 18.36	ACPS
ATOM	273	O	LEU	35	-7.035	25.535	53.466	1.00 17.94	ACPS
ATOM	274	N	ASP	36	-7.049	25.866	51.248	1.00 19.36	ACPS
ATOM	275	CA	ASP	36	-8.419	26.361	51.264	1.00 21.62	ACPS
ATOM	276	CB	ASP	36	-8.866	26.738	49.845	1.00 22.68	ACPS
ATOM	277	CG	ASP	36	-9.949	27.806	49.836	1.00 24.19	ACPS
ATOM	278	OD1	ASP	36	-9.928	28.690	50.724	1.00 25.68	ACPS
ATOM	279	OD2	ASP	36	-10.807	27.773	48.927	1.00 24.47	ACPS
ATOM	280	C	ASP	36	-9.321	25.285	51.857	1.00 22.68	ACPS
ATOM	281	O	ASP	36	-10.269	25.589	52.587	1.00 23.58	ACPS
ATOM	282	N	GLN	37	-9.003	24.024	51.572	1.00 22.62	ACPS
ATOM	283	CA	GLN	37	-9.784	22.899	52.087	1.00 23.62	ACPS
ATOM	284	CB	GLN	37	-9.514	21.653	51.236	1.00 24.76	ACPS
ATOM	285	CG	GLN	37	-9.899	21.812	49.769	1.00 26.90	ACPS
ATOM	286	CD	GLN	37	-9.264	20.761	48.867	1.00 29.15	ACPS
ATOM	287	OE1	GLN	37	-9.409	19.557	49.092	1.00 30.76	ACPS
ATOM	288	NE2	GLN	37	-8.556	21.215	47.836	1.00 30.60	ACPS
ATOM	289	C	GLN	37	-9.445	22.617	53.554	1.00 23.33	ACPS
ATOM	290	O	GLN	37	-10.321	22.331	54.367	1.00 23.90	ACPS
ATOM	291	N	TYR	38	-8.161	22.711	53.876	1.00 22.41	ACPS
ATOM	292	CA	TYR	38	-7.644	22.474	55.222	1.00 22.14	ACPS
ATOM	293	CB	TYR	38	-6.115	22.564	55.169	1.00 20.71	ACPS
ATOM	294	CG	TYR	38	-5.376	22.533	56.491	1.00 20.71	ACPS

FIG. 2A-6

ATOM	295	CD1	TYR	38	-4.945	23.711	57.107	1.00 20.16	ACPS
ATOM	296	CE1	TYR	38	-4.180	23.677	58.276	1.00 21.07	ACPS
ATOM	297	CD2	TYR	38	-5.033	21.322	57.084	1.00 19.25	ACPS
ATOM	298	CE2	TYR	38	-4.275	21.276	58.246	1.00 20.56	ACPS
ATOM	299	CZ	TYR	38	-3.848	22.451	58.837	1.00 21.15	ACPS
ATOM	300	OH	TYR	38	-3.079	22.392	59.976	1.00 21.86	ACPS
ATOM	301	C	TYR	38	-8.191	23.441	56.270	1.00 22.57	ACPS
ATOM	302	O	TYR	38	-8.599	23.031	57.357	1.00 21.64	ACPS
ATOM	303	N	TYR	39	-8.201	24.727	55.933	1.00 23.00	ACPS
ATOM	304	CA	TYR	39	-8.669	25.750	56.854	1.00 23.93	ACPS
ATOM	305	CB	TYR	39	-8.540	27.139	56.212	1.00 24.42	ACPS
ATOM	306	CG	TYR	39	-7.117	27.588	55.948	1.00 25.39	ACPS
ATOM	307	CD1	TYR	39	-6.061	27.134	56.734	1.00 26.23	ACPS
ATOM	308	CE1	TYR	39	-4.763	27.590	56.525	1.00 27.45	ACPS
ATOM	309	CD2	TYR	39	-6.836	28.512	54.939	1.00 26.81	ACPS
ATOM	310	CE2	TYR	39	-5.540	28.979	54.726	1.00 26.80	ACPS
ATOM	311	CZ	TYR	39	-4.508	28.516	55.522	1.00 27.95	ACPS
ATOM	312	OH	TYR	39	-3.224	28.999	55.337	1.00 28.86	ACPS
ATOM	313	C	TYR	39	-10.095	25.568	57.369	1.00 24.48	ACPS
ATOM	314	O	TYR	39	-10.440	26.118	58.412	1.00 25.01	ACPS
ATOM	315	N	GLU	40	-10.916	24.802	56.656	1.00 24.88	ACPS
ATOM	316	CA	GLU	40	-12.307	24.591	57.067	1.00 26.05	ACPS
ATOM	317	CB	GLU	40	-13.180	24.249	55.854	1.00 27.82	ACPS
ATOM	318	CG	GLU	40	-13.036	25.174	54.661	1.00 30.61	ACPS
ATOM	319	CD	GLU	40	-14.017	24.833	53.551	1.00 31.77	ACPS
ATOM	320	OE1	GLU	40	-14.101	23.640	53.178	1.00 32.73	ACPS
ATOM	321	OE2	GLU	40	-14.697	25.756	53.050	1.00 33.34	ACPS
ATOM	322	C	GLU	40	-12.487	23.467	58.086	1.00 25.59	ACPS
ATOM	323	O	GLU	40	-13.581	23.280	58.618	1.00 26.05	ACPS
ATOM	324	N	LEU	41	-11.420	22.731	58.368	1.00 24.07	ACPS
ATOM	325	CA	LEU	41	-11.509	21.584	59.266	1.00 22.24	ACPS
ATOM	326	CB	LEU	41	-10.578	20.486	58.744	1.00 21.78	ACPS
ATOM	327	CG	LEU	41	-10.760	20.090	57.273	1.00 21.91	ACPS
ATOM	328	CD1	LEU	41	-9.666	19.107	56.881	1.00 21.70	ACPS
ATOM	329	CD2	LEU	41	-12.126	19.474	57.058	1.00 22.12	ACPS
ATOM	330	C	LEU	41	-11.230	21.813	60.748	1.00 21.46	ACPS
ATOM	331	O	LEU	41	-10.614	22.800	61.141	1.00 21.25	ACPS
ATOM	332	N	SER	42	-11.693	20.873	61.567	1.00 21.01	ACPS
ATOM	333	CA	SER	42	-11.476	20.926	63.009	1.00 20.67	ACPS
ATOM	334	CB	SER	42	-12.319	19.865	63.716	1.00 21.24	ACPS
ATOM	335	OG	SER	42	-11.874	18.558	63.388	1.00 20.80	ACPS
ATOM	336	C	SER	42	-10.008	20.617	63.245	1.00 20.69	ACPS
ATOM	337	O	SER	42	-9.309	20.184	62.328	1.00 19.86	ACPS
ATOM	338	N	GLU	43	-9.540	20.834	64.469	1.00 19.62	ACPS
ATOM	339	CA	GLU	43	-8.146	20.568	64.815	1.00 19.23	ACPS
ATOM	340	CB	GLU	43	-7.932	20.830	66.312	1.00 20.39	ACPS
ATOM	341	CG	GLU	43	-6.524	20.541	66.843	1.00 22.14	ACPS
ATOM	342	CD	GLU	43	-6.452	20.617	68.366	1.00 23.47	ACPS
ATOM	343	OE1	GLU	43	-6.731	21.698	68.922	1.00 23.93	ACPS
ATOM	344	OE2	GLU	43	-6.118	19.594	69.004	1.00 24.66	ACPS
ATOM	345	C	GLU	43	-7.789	19.120	64.473	1.00 18.65	ACPS
ATOM	346	O	GLU	43	-6.755	18.849	63.864	1.00 18.62	ACPS
ATOM	347	N	LYS	44	-8.653	18.190	64.853	1.00 17.32	ACPS
ATOM	348	CA	LYS	44	-8.403	16.777	64.591	1.00 17.24	ACPS
ATOM	349	CB	LYS	44	-9.441	15.931	65.326	1.00 16.54	ACPS
ATOM	350	CG	LYS	44	-9.404	14.452	64.984	1.00 17.99	ACPS
ATOM	351	CD	LYS	44	-10.561	13.732	65.664	1.00 19.56	ACPS

FIG. 2A-7


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ATOM    352  CE  LYS    44     -10.691  12.285  65.205  1.00 19.17      ACPS
ATOM    353  NZ  LYS    44     -11.159  12.153  63.799  1.00 19.63      ACPS
ATOM    354  C   LYS    44      -8.413  16.431  63.099  1.00 16.56      ACPS
ATOM    355  O   LYS    44      -7.530  15.719  62.613  1.00 16.25      ACPS
ATOM    356  N   ARG    45      -9.412  16.923  62.375  1.00 16.89      ACPS
ATOM    357  CA  ARG    45      -9.507  16.641  60.947  1.00 17.08      ACPS
ATOM    358  CB  ARG    45     -10.849  17.131  60.400  1.00 19.32      ACPS
ATOM    359  CG  ARG    45     -12.053  16.345  60.910  1.00 21.73      ACPS
ATOM    360  CD  ARG    45     -12.092  14.927  60.336  1.00 25.16      ACPS
ATOM    361  NE  ARG    45     -13.304  14.213  60.741  1.00 28.95      ACPS
ATOM    362  CZ  ARG    45     -13.616  12.977  60.360  1.00 30.49      ACPS
ATOM    363  NH1 ARG    45     -14.743  12.419  60.783  1.00 31.89      ACPS
ATOM    364  NH2 ARG    45     -12.808  12.296  59.553  1.00 32.45      ACPS
ATOM    365  C   ARG    45      -8.353  17.284  60.189  1.00 16.29      ACPS
ATOM    366  O   ARG    45      -7.871  16.734  59.198  1.00 15.72      ACPS
ATOM    367  N   LYS    46      -7.917  18.455  60.644  1.00 15.52      ACPS
ATOM    368  CA  LYS    46      -6.796  19.128  60.009  1.00 15.32      ACPS
ATOM    369  CB  LYS    46      -6.449  20.429  60.746  1.00 15.53      ACPS
ATOM    370  CG  LYS    46      -7.232  21.666  60.320  1.00 18.65      ACPS
ATOM    371  CD  LYS    46      -6.678  22.887  61.051  1.00 20.77      ACPS
ATOM    372  CE  LYS    46      -7.201  24.203  60.485  1.00 22.56      ACPS
ATOM    373  NZ  LYS    46      -8.661  24.396  60.688  1.00 24.62      ACPS
ATOM    374  C   LYS    46      -5.584  18.207  60.036  1.00 14.61      ACPS
ATOM    375  O   LYS    46      -4.892  18.051  59.033  1.00 14.78      ACPS
ATOM    376  N   ASN    47      -5.320  17.602  61.190  1.00 14.97      ACPS
ATOM    377  CA  ASN    47      -4.174  16.711  61.329  1.00 14.85      ACPS
ATOM    378  CB  ASN    47      -4.064  16.233  62.783  1.00 16.85      ACPS
ATOM    379  CG  ASN    47      -2.877  15.317  63.008  1.00 19.82      ACPS
ATOM    380  OD1 ASN    47      -1.732  15.704  62.794  1.00 22.35      ACPS
ATOM    381  ND2 ASN    47      -3.149  14.093  63.439  1.00 21.62      ACPS
ATOM    382  C   ASN    47      -4.283  15.517  60.373  1.00 14.22      ACPS
ATOM    383  O   ASN    47      -3.312  15.159  59.702  1.00 13.37      ACPS
ATOM    384  N   GLU    48      -5.461  14.915  60.289  1.00 13.02      ACPS
ATOM    385  CA  GLU    48      -5.650  13.774  59.392  1.00 13.33      ACPS
ATOM    386  CB  GLU    48      -7.005  13.122  59.666  1.00 13.97      ACPS
ATOM    387  CG  GLU    48      -7.094  12.540  61.075  1.00 17.87      ACPS
ATOM    388  CD  GLU    48      -8.518  12.306  61.525  1.00 19.35      ACPS
ATOM    389  OE1 GLU    48      -8.699  11.814  62.657  1.00 22.50      ACPS
ATOM    390  OE2 GLU    48      -9.449  12.615  60.754  1.00 22.51      ACPS
ATOM    391  C   GLU    48      -5.531  14.180  57.925  1.00 12.99      ACPS
ATOM    392  O   GLU    48      -4.927  13.463  57.121  1.00 12.41      ACPS
ATOM    393  N   PHE    49      -6.098  15.331  57.573  1.00 12.16      ACPS
ATOM    394  CA  PHE    49      -6.015  15.818  56.204  1.00 11.74      ACPS
ATOM    395  CB  PHE    49      -6.827  17.118  56.058  1.00 12.28      ACPS
ATOM    396  CG  PHE    49      -6.785  17.716  54.674  1.00 13.38      ACPS
ATOM    397  CD1 PHE    49      -7.742  17.379  53.724  1.00 13.30      ACPS
ATOM    398  CD2 PHE    49      -5.794  18.626  54.324  1.00 12.58      ACPS
ATOM    399  CE1 PHE    49      -7.710  17.950  52.449  1.00 14.47      ACPS
ATOM    400  CE2 PHE    49      -5.754  19.197  53.058  1.00 13.76      ACPS
ATOM    401  CZ  PHE    49      -6.714  18.860  52.120  1.00 14.53      ACPS
ATOM    402  C   PHE    49      -4.549  16.076  55.846  1.00 11.65      ACPS
ATOM    403  O   PHE    49      -4.059  15.616  54.809  1.00 11.61      ACPS
ATOM    404  N   LEU    50      -3.852  16.805  56.717  1.00 11.42      ACPS
ATOM    405  CA  LEU    50      -2.454  17.140  56.489  1.00 11.53      ACPS
ATOM    406  CB  LEU    50      -1.947  18.075  57.597  1.00 12.38      ACPS
ATOM    407  CG  LEU    50      -0.473  18.512  57.597  1.00 12.32      ACPS
ATOM    408  CD1 LEU    50      -0.131  19.277  56.323  1.00 14.40      ACPS
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FIG. 2A-8

ATOM	409	CD2	LEU	50	-0.213	19.390	58.824	1.00	13.78	ACPS
ATOM	410	C	LEU	50	-1.573	15.900	56.413	1.00	10.56	ACPS
ATOM	411	O	LEU	50	-0.684	15.827	55.569	1.00	10.55	ACPS
ATOM	412	N	ALA	51	-1.806	14.936	57.301	1.00	10.65	ACPS
ATOM	413	CA	ALA	51	-1.001	13.711	57.291	1.00	10.86	ACPS
ATOM	414	CB	ALA	51	-1.330	12.847	58.510	1.00	10.65	ACPS
ATOM	415	C	ALA	51	-1.213	12.905	56.003	1.00	11.03	ACPS
ATOM	416	O	ALA	51	-0.274	12.296	55.481	1.00	10.16	ACPS
ATOM	417	N	GLY	52	-2.441	12.913	55.490	1.00	11.30	ACPS
ATOM	418	CA	GLY	52	-2.742	12.186	54.267	1.00	11.27	ACPS
ATOM	419	C	GLY	52	-2.113	12.848	53.050	1.00	11.12	ACPS
ATOM	420	O	GLY	52	-1.635	12.174	52.144	1.00	10.32	ACPS
ATOM	421	N	ARG	53	-2.118	14.177	53.026	1.00	10.73	ACPS
ATOM	422	CA	ARG	53	-1.521	14.896	51.906	1.00	10.83	ACPS
ATOM	423	CB	ARG	53	-1.919	16.385	51.943	1.00	11.05	ACPS
ATOM	424	CG	ARG	53	-3.089	16.756	51.012	1.00	13.36	ACPS
ATOM	425	CD	ARG	53	-4.316	15.894	51.232	1.00	14.65	ACPS
ATOM	426	NE	ARG	53	-5.419	16.229	50.322	1.00	13.75	ACPS
ATOM	427	CZ	ARG	53	-6.569	15.562	50.280	1.00	14.79	ACPS
ATOM	428	NH1	ARG	53	-6.761	14.525	51.087	1.00	14.78	ACPS
ATOM	429	NH2	ARG	53	-7.534	15.932	49.445	1.00	15.39	ACPS
ATOM	430	C	ARG	53	0.001	14.732	51.974	1.00	10.44	ACPS
ATOM	431	O	ARG	53	0.654	14.603	50.938	1.00	10.68	ACPS
ATOM	432	N	PHE	54	0.557	14.728	53.193	1.00	10.64	ACPS
ATOM	433	CA	PHE	54	1.999	14.549	53.396	1.00	9.72	ACPS
ATOM	434	CB	PHE	54	2.308	14.710	54.903	1.00	10.85	ACPS
ATOM	435	CG	PHE	54	3.770	14.621	55.264	1.00	11.55	ACPS
ATOM	436	CD1	PHE	54	4.397	13.386	55.407	1.00	12.45	ACPS
ATOM	437	CD2	PHE	54	4.505	15.780	55.522	1.00	12.56	ACPS
ATOM	438	CE1	PHE	54	5.729	13.301	55.806	1.00	12.31	ACPS
ATOM	439	CE2	PHE	54	5.841	15.709	55.923	1.00	11.84	ACPS
ATOM	440	CZ	PHE	54	6.452	14.462	56.066	1.00	13.57	ACPS
ATOM	441	C	PHE	54	2.392	13.154	52.861	1.00	9.79	ACPS
ATOM	442	O	PHE	54	3.377	13.010	52.123	1.00	9.57	ACPS
ATOM	443	N	ALA	55	1.607	12.136	53.210	1.00	9.67	ACPS
ATOM	444	CA	ALA	55	1.873	10.770	52.742	1.00	9.05	ACPS
ATOM	445	CB	ALA	55	0.894	9.788	53.396	1.00	9.23	ACPS
ATOM	446	C	ALA	55	1.758	10.694	51.218	1.00	9.72	ACPS
ATOM	447	O	ALA	55	2.578	10.070	50.550	1.00	10.39	ACPS
ATOM	448	N	ALA	56	0.730	11.327	50.666	1.00	9.39	ACPS
ATOM	449	CA	ALA	56	0.550	11.313	49.215	1.00	9.78	ACPS
ATOM	450	CB	ALA	56	-0.759	12.014	48.846	1.00	10.10	ACPS
ATOM	451	C	ALA	56	1.728	11.969	48.487	1.00	9.83	ACPS
ATOM	452	O	ALA	56	2.158	11.479	47.451	1.00	10.05	ACPS
ATOM	453	N	LYS	57	2.242	13.077	49.026	1.00	9.72	ACPS
ATOM	454	CA	LYS	57	3.361	13.758	48.388	1.00	10.49	ACPS
ATOM	455	CB	LYS	57	3.477	15.194	48.914	1.00	9.29	ACPS
ATOM	456	CG	LYS	57	2.243	16.015	48.546	1.00	9.85	ACPS
ATOM	457	CD	LYS	57	2.383	17.492	48.881	1.00	10.42	ACPS
ATOM	458	CE	LYS	57	1.057	18.196	48.628	1.00	10.41	ACPS
ATOM	459	NZ	LYS	57	1.214	19.689	48.629	1.00	10.56	ACPS
ATOM	460	C	LYS	57	4.668	12.986	48.549	1.00	10.05	ACPS
ATOM	461	O	LYS	57	5.501	12.992	47.632	1.00	11.38	ACPS
ATOM	462	N	GLU	58	4.863	12.322	49.687	1.00	10.76	ACPS
ATOM	463	CA	GLU	58	6.073	11.513	49.846	1.00	10.03	ACPS
ATOM	464	CB	GLU	58	6.270	11.064	51.304	1.00	10.79	ACPS
ATOM	465	CG	GLU	58	6.674	12.221	52.234	1.00	12.67	ACPS

FIG. 2A-9

ATOM	466	CD	GLU	58	7.551	11.800	53.407	1.00 14.43	ACPS
ATOM	467	OE1	GLU	58	7.452	10.642	53.851	1.00 12.52	ACPS
ATOM	468	OE2	GLU	58	8.343	12.641	53.905	1.00 14.76	ACPS
ATOM	469	C	GLU	58	5.969	10.307	48.903	1.00 10.19	ACPS
ATOM	470	O	GLU	58	6.960	9.897	48.298	1.00 11.04	ACPS
ATOM	471	N	ALA	59	4.773	9.742	48.765	1.00 10.50	ACPS
ATOM	472	CA	ALA	59	4.596	8.622	47.844	1.00 10.19	ACPS
ATOM	473	CB	ALA	59	3.178	8.031	47.965	1.00 9.73	ACPS
ATOM	474	C	ALA	59	4.866	9.100	46.415	1.00 11.21	ACPS
ATOM	475	O	ALA	59	5.510	8.402	45.641	1.00 11.07	ACPS
ATOM	476	N	PHE	60	4.377	10.289	46.071	1.00 10.97	ACPS
ATOM	477	CA	PHE	60	4.614	10.824	44.735	1.00 11.41	ACPS
ATOM	478	CB	PHE	60	3.918	12.182	44.536	1.00 11.35	ACPS
ATOM	479	CG	PHE	60	4.213	12.810	43.191	1.00 11.93	ACPS
ATOM	480	CD1	PHE	60	3.492	12.439	42.057	1.00 11.51	ACPS
ATOM	481	CD2	PHE	60	5.284	13.684	43.047	1.00 11.60	ACPS
ATOM	482	CE1	PHE	60	3.841	12.926	40.793	1.00 12.57	ACPS
ATOM	483	CE2	PHE	60	5.641	14.174	41.794	1.00 12.35	ACPS
ATOM	484	CZ	PHE	60	4.921	13.794	40.671	1.00 11.51	ACPS
ATOM	485	C	PHE	60	6.109	11.014	44.481	1.00 10.91	ACPS
ATOM	486	O	PHE	60	6.599	10.703	43.390	1.00 11.17	ACPS
ATOM	487	N	SER	61	6.828	11.529	45.483	1.00 11.07	ACPS
ATOM	488	CA	SER	61	8.262	11.775	45.336	1.00 11.40	ACPS
ATOM	489	CB	SER	61	8.815	12.510	46.561	1.00 11.56	ACPS
ATOM	490	OG	SER	61	9.026	11.642	47.660	1.00 12.07	ACPS
ATOM	491	C	SER	61	9.039	10.487	45.094	1.00 12.17	ACPS
ATOM	492	O	SER	61	10.102	10.508	44.476	1.00 11.91	ACPS
ATOM	493	N	LYS	62	8.513	9.365	45.583	1.00 11.76	ACPS
ATOM	494	CA	LYS	62	9.165	8.081	45.361	1.00 11.72	ACPS
ATOM	495	CB	LYS	62	8.687	7.051	46.395	1.00 9.91	ACPS
ATOM	496	CG	LYS	62	9.172	7.377	47.836	1.00 10.07	ACPS
ATOM	497	CD	LYS	62	8.584	6.402	48.888	1.00 8.91	ACPS
ATOM	498	CE	LYS	62	8.901	6.838	50.320	1.00 10.72	ACPS
ATOM	499	NZ	LYS	62	8.292	5.910	51.344	1.00 10.83	ACPS
ATOM	500	C	LYS	62	8.875	7.603	43.935	1.00 11.87	ACPS
ATOM	501	O	LYS	62	9.758	7.062	43.264	1.00 12.36	ACPS
ATOM	502	N	ALA	63	7.642	7.815	43.472	1.00 12.11	ACPS
ATOM	503	CA	ALA	63	7.266	7.408	42.119	1.00 12.83	ACPS
ATOM	504	CB	ALA	63	5.751	7.567	41.914	1.00 11.67	ACPS
ATOM	505	C	ALA	63	8.033	8.259	41.105	1.00 13.18	ACPS
ATOM	506	O	ALA	63	8.402	7.774	40.037	1.00 13.32	ACPS
ATOM	507	N	PHE	64	8.262	9.523	41.457	1.00 13.48	ACPS
ATOM	508	CA	PHE	64	8.987	10.491	40.628	1.00 14.82	ACPS
ATOM	509	CB	PHE	64	8.856	11.878	41.290	1.00 14.97	ACPS
ATOM	510	CG	PHE	64	9.339	13.026	40.451	1.00 17.08	ACPS
ATOM	511	CD1	PHE	64	8.715	13.350	39.253	1.00 17.78	ACPS
ATOM	512	CD2	PHE	64	10.402	13.809	40.885	1.00 17.57	ACPS
ATOM	513	CE1	PHE	64	9.148	14.450	38.495	1.00 18.78	ACPS
ATOM	514	CE2	PHE	64	10.838	14.904	40.137	1.00 18.89	ACPS
ATOM	515	CZ	PHE	64	10.209	15.221	38.944	1.00 18.36	ACPS
ATOM	516	C	PHE	64	10.456	10.048	40.545	1.00 14.87	ACPS
ATOM	517	O	PHE	64	11.136	10.290	39.547	1.00 16.68	ACPS
ATOM	518	N	GLY	65	10.941	9.423	41.615	1.00 14.73	ACPS
ATOM	519	CA	GLY	65	12.302	8.907	41.652	1.00 14.56	ACPS
ATOM	520	C	GLY	65	13.370	9.729	42.351	1.00 14.92	ACPS
ATOM	521	O	GLY	65	14.542	9.351	42.348	1.00 15.63	ACPS
ATOM	522	N	THR	66	12.979	10.826	42.980	1.00 16.03	ACPS

FIG. 2A-10

ATOM	523	CA	THR	66	13.945	11.700	43.643	1.00	16.17	ACPS
ATOM	524	CB	THR	66	13.908	13.103	43.038	1.00	17.57	ACPS
ATOM	525	OG1	THR	66	12.622	13.685	43.290	1.00	16.98	ACPS
ATOM	526	CG2	THR	66	14.150	13.056	41.531	1.00	18.71	ACPS
ATOM	527	C	THR	66	13.770	11.912	45.140	1.00	15.80	ACPS
ATOM	528	O	THR	66	14.713	12.315	45.825	1.00	15.38	ACPS
ATOM	529	N	GLY	67	12.572	11.652	45.649	1.00	15.62	ACPS
ATOM	530	CA	GLY	67	12.319	11.918	47.052	1.00	15.38	ACPS
ATOM	531	C	GLY	67	12.088	13.421	47.173	1.00	15.61	ACPS
ATOM	532	O	GLY	67	12.160	14.137	46.170	1.00	15.25	ACPS
ATOM	533	N	ILE	68	11.801	13.906	48.380	1.00	15.09	ACPS
ATOM	534	CA	ILE	68	11.580	15.332	48.598	1.00	16.65	ACPS
ATOM	535	CB	ILE	68	10.578	15.590	49.762	1.00	15.30	ACPS
ATOM	536	CG2	ILE	68	10.508	17.089	50.063	1.00	16.62	ACPS
ATOM	537	CG1	ILE	68	9.182	15.049	49.413	1.00	14.84	ACPS
ATOM	538	CD1	ILE	68	8.484	15.785	48.269	1.00	15.16	ACPS
ATOM	539	C	ILE	68	12.927	15.967	48.945	1.00	17.33	ACPS
ATOM	540	O	ILE	68	13.610	15.520	49.862	1.00	18.29	ACPS
ATOM	541	N	GLY	69	13.305	17.002	48.202	1.00	18.32	ACPS
ATOM	542	CA	GLY	69	14.574	17.663	48.436	1.00	20.27	ACPS
ATOM	543	C	GLY	69	14.877	18.700	47.371	1.00	20.85	ACPS
ATOM	544	O	GLY	69	13.990	19.447	46.949	1.00	20.98	ACPS
ATOM	545	N	ALA	70	16.128	18.734	46.920	1.00	22.02	ACPS
ATOM	546	CA	ALA	70	16.564	19.710	45.922	1.00	22.94	ACPS
ATOM	547	CB	ALA	70	18.064	19.575	45.690	1.00	24.19	ACPS
ATOM	548	C	ALA	70	15.834	19.655	44.582	1.00	23.39	ACPS
ATOM	549	O	ALA	70	15.623	20.688	43.950	1.00	24.35	ACPS
ATOM	550	N	GLN	71	15.446	18.457	44.153	1.00	22.46	ACPS
ATOM	551	CA	GLN	71	14.765	18.289	42.871	1.00	21.53	ACPS
ATOM	552	CB	GLN	71	15.204	16.971	42.223	1.00	23.55	ACPS
ATOM	553	CG	GLN	71	16.683	16.924	41.843	1.00	26.32	ACPS
ATOM	554	CD	GLN	71	17.185	15.512	41.591	1.00	28.10	ACPS
ATOM	555	OE1	GLN	71	17.349	14.722	42.523	1.00	29.41	ACPS
ATOM	556	NE2	GLN	71	17.435	15.188	40.326	1.00	29.15	ACPS
ATOM	557	C	GLN	71	13.239	18.334	42.931	1.00	20.50	ACPS
ATOM	558	O	GLN	71	12.580	18.424	41.891	1.00	20.08	ACPS
ATOM	559	N	LEU	72	12.668	18.287	44.132	1.00	18.34	ACPS
ATOM	560	CA	LEU	72	11.210	18.292	44.261	1.00	16.54	ACPS
ATOM	561	CB	LEU	72	10.671	16.868	44.034	1.00	16.42	ACPS
ATOM	562	CG	LEU	72	9.146	16.682	44.035	1.00	15.69	ACPS
ATOM	563	CD1	LEU	72	8.539	17.358	42.815	1.00	16.49	ACPS
ATOM	564	CD2	LEU	72	8.811	15.186	44.032	1.00	16.39	ACPS
ATOM	565	C	LEU	72	10.752	18.786	45.632	1.00	15.95	ACPS
ATOM	566	O	LEU	72	11.177	18.260	46.654	1.00	16.86	ACPS
ATOM	567	N	SER	73	9.879	19.789	45.649	1.00	15.85	ACPS
ATOM	568	CA	SER	73	9.360	20.337	46.901	1.00	15.02	ACPS
ATOM	569	CB	SER	73	9.400	21.872	46.865	1.00	16.69	ACPS
ATOM	570	OG	SER	73	8.552	22.454	47.851	1.00	18.22	ACPS
ATOM	571	C	SER	73	7.920	19.896	47.122	1.00	13.98	ACPS
ATOM	572	O	SER	73	7.227	19.531	46.175	1.00	14.35	ACPS
ATOM	573	N	PHE	74	7.469	19.926	48.373	1.00	13.59	ACPS
ATOM	574	CA	PHE	74	6.083	19.584	48.674	1.00	12.78	ACPS
ATOM	575	CB	PHE	74	5.802	19.731	50.177	1.00	12.70	ACPS
ATOM	576	CG	PHE	74	6.274	18.566	51.010	1.00	13.35	ACPS
ATOM	577	CD1	PHE	74	5.663	17.320	50.894	1.00	14.16	ACPS
ATOM	578	CD2	PHE	74	7.308	18.723	51.928	1.00	15.36	ACPS
ATOM	579	CE1	PHE	74	6.071	16.246	51.679	1.00	13.54	ACPS

FIG. 2A-11

ATOM	580	CE2	PHE	74	7.727	17.653	52.720	1.00	14.73	ACPS
ATOM	581	CZ	PHE	74	7.104	16.412	52.592	1.00	14.61	ACPS
ATOM	582	C	PHE	74	5.172	20.539	47.894	1.00	13.25	ACPS
ATOM	583	O	PHE	74	4.070	20.179	47.500	1.00	13.15	ACPS
ATOM	584	N	GLN	75	5.642	21.764	47.665	1.00	13.41	ACPS
ATOM	585	CA	GLN	75	4.848	22.749	46.929	1.00	13.12	ACPS
ATOM	586	CB	GLN	75	5.437	24.152	47.124	1.00	13.58	ACPS
ATOM	587	CG	GLN	75	5.338	24.667	48.545	1.00	14.20	ACPS
ATOM	588	CD	GLN	75	3.897	24.841	48.976	1.00	15.83	ACPS
ATOM	589	OE1	GLN	75	3.077	25.355	48.217	1.00	17.10	ACPS
ATOM	590	NE2	GLN	75	3.581	24.421	50.194	1.00	15.26	ACPS
ATOM	591	C	GLN	75	4.701	22.473	45.430	1.00	13.39	ACPS
ATOM	592	O	GLN	75	3.865	23.097	44.769	1.00	14.75	ACPS
ATOM	593	N	ASP	76	5.502	21.555	44.889	1.00	13.51	ACPS
ATOM	594	CA	ASP	76	5.423	21.214	43.464	1.00	13.36	ACPS
ATOM	595	CB	ASP	76	6.760	20.670	42.950	1.00	14.98	ACPS
ATOM	596	CG	ASP	76	7.907	21.644	43.108	1.00	15.83	ACPS
ATOM	597	OD1	ASP	76	7.682	22.872	43.049	1.00	17.92	ACPS
ATOM	598	OD2	ASP	76	9.049	21.168	43.265	1.00	16.55	ACPS
ATOM	599	C	ASP	76	4.369	20.143	43.177	1.00	13.18	ACPS
ATOM	600	O	ASP	76	4.138	19.781	42.016	1.00	13.17	ACPS
ATOM	601	N	ILE	77	3.743	19.637	44.234	1.00	12.89	ACPS
ATOM	602	CA	ILE	77	2.765	18.561	44.116	1.00	12.84	ACPS
ATOM	603	CB	ILE	77	3.248	17.339	44.932	1.00	11.96	ACPS
ATOM	604	CG2	ILE	77	2.405	16.122	44.608	1.00	11.88	ACPS
ATOM	605	CG1	ILE	77	4.722	17.053	44.638	1.00	12.24	ACPS
ATOM	606	CD1	ILE	77	5.413	16.211	45.724	1.00	12.11	ACPS
ATOM	607	C	ILE	77	1.414	18.999	44.664	1.00	12.77	ACPS
ATOM	608	O	ILE	77	1.330	19.552	45.766	1.00	13.68	ACPS
ATOM	609	N	GLU	78	0.349	18.748	43.910	1.00	12.53	ACPS
ATOM	610	CA	GLU	78	-0.975	19.130	44.373	1.00	12.16	ACPS
ATOM	611	CB	GLU	78	-1.472	20.350	43.587	1.00	12.59	ACPS
ATOM	612	CG	GLU	78	-2.722	20.983	44.167	1.00	13.40	ACPS
ATOM	613	CD	GLU	78	-2.987	22.339	43.559	1.00	14.46	ACPS
ATOM	614	OE1	GLU	78	-3.631	22.398	42.489	1.00	16.38	ACPS
ATOM	615	OE2	GLU	78	-2.524	23.340	44.147	1.00	15.90	ACPS
ATOM	616	C	GLU	78	-1.999	18.014	44.252	1.00	11.56	ACPS
ATOM	617	O	GLU	78	-2.145	17.402	43.198	1.00	12.82	ACPS
ATOM	618	N	ILE	79	-2.704	17.748	45.344	1.00	11.82	ACPS
ATOM	619	CA	ILE	79	-3.750	16.734	45.329	1.00	12.32	ACPS
ATOM	620	CB	ILE	79	-3.893	16.000	46.698	1.00	12.41	ACPS
ATOM	621	CG2	ILE	79	-5.201	15.191	46.723	1.00	12.50	ACPS
ATOM	622	CG1	ILE	79	-2.737	15.010	46.913	1.00	11.83	ACPS
ATOM	623	CD1	ILE	79	-1.372	15.660	47.132	1.00	12.95	ACPS
ATOM	624	C	ILE	79	-5.053	17.483	45.048	1.00	12.37	ACPS
ATOM	625	O	ILE	79	-5.389	18.439	45.747	1.00	13.01	ACPS
ATOM	626	N	ARG	80	-5.753	17.059	44.003	1.00	12.18	ACPS
ATOM	627	CA	ARG	80	-7.037	17.649	43.633	1.00	13.15	ACPS
ATOM	628	CB	ARG	80	-6.981	18.219	42.205	1.00	13.40	ACPS
ATOM	629	CG	ARG	80	-5.887	19.278	41.989	1.00	14.66	ACPS
ATOM	630	CD	ARG	80	-5.931	19.884	40.592	1.00	16.60	ACPS
ATOM	631	NE	ARG	80	-4.846	20.849	40.396	1.00	16.81	ACPS
ATOM	632	CZ	ARG	80	-4.588	21.471	39.248	1.00	18.53	ACPS
ATOM	633	NH1	ARG	80	-3.581	22.331	39.175	1.00	18.94	ACPS
ATOM	634	NH2	ARG	80	-5.331	21.240	38.173	1.00	17.96	ACPS
ATOM	635	C	ARG	80	-8.061	16.516	43.701	1.00	13.09	ACPS
ATOM	636	O	ARG	80	-7.697	15.352	43.882	1.00	13.74	ACPS

FIG. 2A-12

ATOM	637	N	LYS	81	-9.339	16.837	43.577	1.00 13.78	ACPS
ATOM	638	CA	LYS	81	-10.349	15.789	43.610	1.00 15.56	ACPS
ATOM	639	CB	LYS	81	-10.943	15.648	45.017	1.00 17.86	ACPS
ATOM	640	CG	LYS	81	-11.693	16.852	45.502	1.00 21.01	ACPS
ATOM	641	CD	LYS	81	-12.183	16.669	46.939	1.00 23.45	ACPS
ATOM	642	CE	LYS	81	-12.982	17.886	47.415	1.00 25.03	ACPS
ATOM	643	NZ	LYS	81	-13.413	17.764	48.847	1.00 28.19	ACPS
ATOM	644	C	LYS	81	-11.446	16.080	42.612	1.00 15.29	ACPS
ATOM	645	O	LYS	81	-11.752	17.249	42.329	1.00 15.96	ACPS
ATOM	646	N	ASP	82	-12.025	15.019	42.060	1.00 14.49	ACPS
ATOM	647	CA	ASP	82	-13.102	15.191	41.102	1.00 13.96	ACPS
ATOM	648	CB	ASP	82	-13.140	14.042	40.067	1.00 14.55	ACPS
ATOM	649	CG	ASP	82	-13.516	12.682	40.660	1.00 14.41	ACPS
ATOM	650	OD1	ASP	82	-14.130	12.609	41.738	1.00 13.41	ACPS
ATOM	651	OD2	ASP	82	-13.199	11.666	40.003	1.00 16.39	ACPS
ATOM	652	C	ASP	82	-14.440	15.347	41.816	1.00 14.59	ACPS
ATOM	653	O	ASP	82	-14.506	15.366	43.048	1.00 13.66	ACPS
ATOM	654	N	GLN	83	-15.506	15.464	41.038	1.00 16.21	ACPS
ATOM	655	CA	GLN	83	-16.836	15.671	41.596	1.00 18.34	ACPS
ATOM	656	CB	GLN	83	-17.809	15.984	40.454	1.00 20.79	ACPS
ATOM	657	CG	GLN	83	-17.344	17.201	39.649	1.00 25.58	ACPS
ATOM	658	CD	GLN	83	-18.065	17.378	38.327	1.00 28.04	ACPS
ATOM	659	OE1	GLN	83	-17.669	18.207	37.505	1.00 30.79	ACPS
ATOM	660	NE2	GLN	83	-19.130	16.606	38.114	1.00 29.51	ACPS
ATOM	661	C	GLN	83	-17.351	14.530	42.465	1.00 18.31	ACPS
ATOM	662	O	GLN	83	-18.304	14.707	43.225	1.00 18.85	ACPS
ATOM	663	N	ASN	84	-16.722	13.366	42.363	1.00 18.00	ACPS
ATOM	664	CA	ASN	84	-17.126	12.220	43.178	1.00 18.03	ACPS
ATOM	665	CB	ASN	84	-16.984	10.901	42.414	1.00 19.80	ACPS
ATOM	666	CG	ASN	84	-17.959	10.776	41.269	1.00 21.78	ACPS
ATOM	667	OD1	ASN	84	-19.160	10.993	41.432	1.00 24.79	ACPS
ATOM	668	ND2	ASN	84	-17.451	10.404	40.105	1.00 23.27	ACPS
ATOM	669	C	ASN	84	-16.282	12.111	44.439	1.00 16.61	ACPS
ATOM	670	O	ASN	84	-16.534	11.247	45.276	1.00 16.49	ACPS
ATOM	671	N	GLY	85	-15.278	12.972	44.568	1.00 15.58	ACPS
ATOM	672	CA	GLY	85	-14.424	12.920	45.741	1.00 14.25	ACPS
ATOM	673	C	GLY	85	-13.153	12.107	45.539	1.00 14.48	ACPS
ATOM	674	O	GLY	85	-12.368	11.945	46.475	1.00 14.65	ACPS
ATOM	675	N	LYS	86	-12.941	11.597	44.330	1.00 13.84	ACPS
ATOM	676	CA	LYS	86	-11.741	10.810	44.042	1.00 12.93	ACPS
ATOM	677	CB	LYS	86	-11.911	10.014	42.745	1.00 13.87	ACPS
ATOM	678	CG	LYS	86	-10.672	9.204	42.353	1.00 15.94	ACPS
ATOM	679	CD	LYS	86	-10.789	8.679	40.926	1.00 19.84	ACPS
ATOM	680	CE	LYS	86	-9.548	7.906	40.485	1.00 20.40	ACPS
ATOM	681	NZ	LYS	86	-9.484	6.545	41.078	1.00 21.85	ACPS
ATOM	682	C	LYS	86	-10.534	11.730	43.883	1.00 13.03	ACPS
ATOM	683	O	LYS	86	-10.557	12.660	43.078	1.00 12.98	ACPS
ATOM	684	N	PRO	87	-9.461	11.478	44.647	1.00 11.91	ACPS
ATOM	685	CD	PRO	87	-9.315	10.444	45.694	1.00 12.38	ACPS
ATOM	686	CA	PRO	87	-8.262	12.308	44.551	1.00 11.87	ACPS
ATOM	687	CB	PRO	87	-7.556	12.043	45.874	1.00 10.81	ACPS
ATOM	688	CG	PRO	87	-7.838	10.568	46.090	1.00 11.34	ACPS
ATOM	689	C	PRO	87	-7.386	11.913	43.377	1.00 11.68	ACPS
ATOM	690	O	PRO	87	-7.429	10.768	42.910	1.00 11.62	ACPS
ATOM	691	N	TYR	88	-6.615	12.882	42.895	1.00 11.62	ACPS
ATOM	692	CA	TYR	88	-5.639	12.674	41.830	1.00 11.77	ACPS
ATOM	693	CB	TYR	88	-6.288	12.733	40.432	1.00 13.03	ACPS

FIG. 2A-13

ATOM	694	CG	TYR	88	-6.922	14.047	40.032	1.00 14.02	ACPS
ATOM	695	CD1	TYR	88	-6.188	15.023	39.364	1.00 14.07	ACPS
ATOM	696	CE1	TYR	88	-6.787	16.222	38.963	1.00 14.84	ACPS
ATOM	697	CD2	TYR	88	-8.271	14.298	40.294	1.00 14.32	ACPS
ATOM	698	CE2	TYR	88	-8.877	15.480	39.898	1.00 15.51	ACPS
ATOM	699	CZ	TYR	88	-8.131	16.442	39.232	1.00 15.27	ACPS
ATOM	700	OH	TYR	88	-8.728	17.622	38.835	1.00 17.40	ACPS
ATOM	701	C	TYR	88	-4.571	13.748	42.029	1.00 11.78	ACPS
ATOM	702	O	TYR	88	-4.801	14.752	42.698	1.00 11.93	ACPS
ATOM	703	N	ILE	89	-3.385	13.521	41.487	1.00 11.68	ACPS
ATOM	704	CA	ILE	89	-2.302	14.482	41.647	1.00 12.44	ACPS
ATOM	705	CB	ILE	89	-1.037	13.765	42.199	1.00 11.85	ACPS
ATOM	706	CG2	ILE	89	0.239	14.579	41.910	1.00 11.95	ACPS
ATOM	707	CG1	ILE	89	-1.185	13.538	43.706	1.00 11.65	ACPS
ATOM	708	CD1	ILE	89	-0.021	12.751	44.320	1.00 12.93	ACPS
ATOM	709	C	ILE	89	-1.921	15.214	40.371	1.00 12.52	ACPS
ATOM	710	O	ILE	89	-2.000	14.662	39.271	1.00 13.59	ACPS
ATOM	711	N	ILE	90	-1.527	16.470	40.539	1.00 14.09	ACPS
ATOM	712	CA	ILE	90	-1.036	17.282	39.434	1.00 14.07	ACPS
ATOM	713	CB	ILE	90	-1.937	18.514	39.151	1.00 14.62	ACPS
ATOM	714	CG2	ILE	90	-1.254	19.433	38.127	1.00 15.25	ACPS
ATOM	715	CG1	ILE	90	-3.313	18.067	38.636	1.00 15.67	ACPS
ATOM	716	CD1	ILE	90	-3.289	17.301	37.330	1.00 16.06	ACPS
ATOM	717	C	ILE	90	0.357	17.780	39.855	1.00 14.28	ACPS
ATOM	718	O	ILE	90	0.514	18.342	40.940	1.00 13.87	ACPS
ATOM	719	N	CYS	91	1.362	17.520	39.016	1.00 15.25	ACPS
ATOM	720	CA	CYS	91	2.737	17.974	39.242	1.00 15.44	ACPS
ATOM	721	CB	CYS	91	3.677	16.806	39.561	1.00 15.30	ACPS
ATOM	722	SG	CYS	91	5.404	17.317	39.841	1.00 14.62	ACPS
ATOM	723	C	CYS	91	3.139	18.606	37.916	1.00 16.53	ACPS
ATOM	724	O	CYS	91	3.585	17.926	36.990	1.00 17.19	ACPS
ATOM	725	N	THR	92	2.958	19.912	37.830	1.00 17.43	ACPS
ATOM	726	CA	THR	92	3.255	20.640	36.609	1.00 19.27	ACPS
ATOM	727	CB	THR	92	2.946	22.137	36.804	1.00 20.38	ACPS
ATOM	728	OG1	THR	92	1.550	22.286	37.117	1.00 22.97	ACPS
ATOM	729	CG2	THR	92	3.257	22.920	35.542	1.00 21.13	ACPS
ATOM	730	C	THR	92	4.685	20.436	36.102	1.00 19.66	ACPS
ATOM	731	O	THR	92	4.909	20.405	34.885	1.00 19.81	ACPS
ATOM	732	N	LYS	93	5.641	20.269	37.021	1.00 19.24	ACPS
ATOM	733	CA	LYS	93	7.040	20.049	36.633	1.00 20.40	ACPS
ATOM	734	CB	LYS	93	7.950	19.936	37.869	1.00 21.00	ACPS
ATOM	735	CG	LYS	93	8.283	21.253	38.540	1.00 23.04	ACPS
ATOM	736	CD	LYS	93	9.271	21.044	39.674	1.00 23.13	ACPS
ATOM	737	CE	LYS	93	9.590	22.347	40.394	1.00 25.70	ACPS
ATOM	738	NZ	LYS	93	10.683	22.160	41.393	1.00 27.21	ACPS
ATOM	739	C	LYS	93	7.194	18.774	35.816	1.00 19.95	ACPS
ATOM	740	O	LYS	93	8.155	18.624	35.063	1.00 19.63	ACPS
ATOM	741	N	LEU	94	6.251	17.851	35.978	1.00 20.99	ACPS
ATOM	742	CA	LEU	94	6.279	16.575	35.264	1.00 22.26	ACPS
ATOM	743	CB	LEU	94	5.643	15.485	36.129	1.00 23.41	ACPS
ATOM	744	CG	LEU	94	5.579	14.064	35.563	1.00 24.26	ACPS
ATOM	745	CD1	LEU	94	6.980	13.493	35.405	1.00 26.39	ACPS
ATOM	746	CD2	LEU	94	4.761	13.194	36.507	1.00 25.01	ACPS
ATOM	747	C	LEU	94	5.530	16.674	33.936	1.00 23.14	ACPS
ATOM	748	O	LEU	94	6.110	16.499	32.862	1.00 22.82	ACPS
ATOM	749	N	SER	95	4.234	16.942	34.028	1.00 23.89	ACPS
ATOM	750	CA	SER	95	3.375	17.074	32.861	1.00 25.33	ACPS

FIG. 2A-14

ATOM	751	CB	SER	95	3.268	15.736	32.112	1.00	26.52	ACPS
ATOM	752	OG	SER	95	2.573	14.752	32.861	1.00	27.95	ACPS
ATOM	753	C	SER	95	2.002	17.531	33.354	1.00	25.56	ACPS
ATOM	754	O	SER	95	1.760	17.599	34.561	1.00	24.02	ACPS
ATOM	755	N	PRO	96	1.090	17.874	32.432	1.00	26.00	ACPS
ATOM	756	CD	PRO	96	1.289	18.101	30.986	1.00	26.52	ACPS
ATOM	757	CA	PRO	96	-0.240	18.324	32.853	1.00	25.75	ACPS
ATOM	758	CB	PRO	96	-0.709	19.147	31.657	1.00	26.31	ACPS
ATOM	759	CG	PRO	96	-0.119	18.392	30.506	1.00	26.75	ACPS
ATOM	760	C	PRO	96	-1.201	17.179	33.176	1.00	25.06	ACPS
ATOM	761	O	PRO	96	-2.304	17.414	33.664	1.00	25.74	ACPS
ATOM	762	N	ALA	97	-0.773	15.950	32.907	1.00	24.25	ACPS
ATOM	763	CA	ALA	97	-1.599	14.769	33.142	1.00	23.20	ACPS
ATOM	764	CB	ALA	97	-0.967	13.555	32.479	1.00	24.01	ACPS
ATOM	765	C	ALA	97	-1.872	14.463	34.611	1.00	22.43	ACPS
ATOM	766	O	ALA	97	-1.072	14.786	35.490	1.00	22.83	ACPS
ATOM	767	N	ALA	98	-3.020	13.841	34.865	1.00	21.00	ACPS
ATOM	768	CA	ALA	98	-3.411	13.462	36.215	1.00	19.60	ACPS
ATOM	769	CB	ALA	98	-4.914	13.140	36.259	1.00	19.71	ACPS
ATOM	770	C	ALA	98	-2.597	12.232	36.601	1.00	18.50	ACPS
ATOM	771	O	ALA	98	-2.426	11.313	35.796	1.00	19.87	ACPS
ATOM	772	N	VAL	99	-2.084	12.231	37.826	1.00	15.98	ACPS
ATOM	773	CA	VAL	99	-1.299	11.120	38.346	1.00	14.14	ACPS
ATOM	774	CB	VAL	99	-0.042	11.661	39.041	1.00	15.01	ACPS
ATOM	775	CG1	VAL	99	0.630	10.575	39.854	1.00	15.26	ACPS
ATOM	776	CG2	VAL	99	0.909	12.221	37.990	1.00	14.69	ACPS
ATOM	777	C	VAL	99	-2.192	10.357	39.336	1.00	13.62	ACPS
ATOM	778	O	VAL	99	-2.935	10.971	40.098	1.00	14.19	ACPS
ATOM	779	N	HIS	100	-2.132	9.029	39.306	1.00	12.36	ACPS
ATOM	780	CA	HIS	100	-2.949	8.192	40.178	1.00	12.74	ACPS
ATOM	781	CB	HIS	100	-2.894	6.741	39.708	1.00	13.48	ACPS
ATOM	782	CG	HIS	100	-3.505	6.514	38.362	1.00	14.92	ACPS
ATOM	783	CD2	HIS	100	-2.938	6.353	37.143	1.00	15.96	ACPS
ATOM	784	ND1	HIS	100	-4.868	6.432	38.165	1.00	15.90	ACPS
ATOM	785	CE1	HIS	100	-5.113	6.232	36.883	1.00	17.29	ACPS
ATOM	786	NE2	HIS	100	-3.960	6.181	36.241	1.00	15.85	ACPS
ATOM	787	C	HIS	100	-2.513	8.233	41.630	1.00	12.24	ACPS
ATOM	788	O	HIS	100	-1.328	8.140	41.927	1.00	12.33	ACPS
ATOM	789	N	VAL	101	-3.487	8.363	42.525	1.00	11.72	ACPS
ATOM	790	CA	VAL	101	-3.217	8.365	43.958	1.00	11.15	ACPS
ATOM	791	CB	VAL	101	-2.899	9.811	44.477	1.00	11.69	ACPS
ATOM	792	CG1	VAL	101	-4.142	10.694	44.373	1.00	12.75	ACPS
ATOM	793	CG2	VAL	101	-2.391	9.758	45.924	1.00	12.34	ACPS
ATOM	794	C	VAL	101	-4.430	7.815	44.725	1.00	10.53	ACPS
ATOM	795	O	VAL	101	-5.565	7.914	44.253	1.00	10.71	ACPS
ATOM	796	N	SER	102	-4.174	7.176	45.871	1.00	9.38	ACPS
ATOM	797	CA	SER	102	-5.243	6.698	46.748	1.00	9.83	ACPS
ATOM	798	CB	SER	102	-5.574	5.218	46.517	1.00	10.13	ACPS
ATOM	799	OG	SER	102	-6.713	4.863	47.295	1.00	9.75	ACPS
ATOM	800	C	SER	102	-4.782	6.906	48.192	1.00	9.45	ACPS
ATOM	801	O	SER	102	-3.608	6.730	48.493	1.00	10.30	ACPS
ATOM	802	N	ILE	103	-5.712	7.277	49.071	1.00	9.23	ACPS
ATOM	803	CA	ILE	103	-5.417	7.563	50.474	1.00	9.67	ACPS
ATOM	804	CB	ILE	103	-5.683	9.063	50.774	1.00	9.72	ACPS
ATOM	805	CG2	ILE	103	-5.495	9.382	52.283	1.00	8.94	ACPS
ATOM	806	CG1	ILE	103	-4.778	9.912	49.885	1.00	10.44	ACPS
ATOM	807	CD1	ILE	103	-5.088	11.421	49.938	1.00	11.38	ACPS

FIG. 2A-15

ATOM	808	C	ILE	103	-6.299	6.728	51.388	1.00	9.74	ACPS
ATOM	809	O	ILE	103	-7.447	6.432	51.041	1.00	9.47	ACPS
ATOM	810	N	THR	104	-5.751	6.334	52.541	1.00	9.43	ACPS
ATOM	811	CA	THR	104	-6.507	5.567	53.537	1.00	9.07	ACPS
ATOM	812	CB	THR	104	-6.323	4.034	53.329	1.00	9.49	ACPS
ATOM	813	OG1	THR	104	-7.164	3.312	54.246	1.00	10.14	ACPS
ATOM	814	CG2	THR	104	-4.878	3.617	53.528	1.00	8.69	ACPS
ATOM	815	C	THR	104	-6.067	5.976	54.949	1.00	9.89	ACPS
ATOM	816	O	THR	104	-4.896	6.283	55.174	1.00	9.73	ACPS
ATOM	817	N	HIS	105	-7.006	5.978	55.891	1.00	10.13	ACPS
ATOM	818	CA	HIS	105	-6.734	6.384	57.266	1.00	10.93	ACPS
ATOM	819	CB	HIS	105	-7.632	7.572	57.622	1.00	11.25	ACPS
ATOM	820	CG	HIS	105	-7.371	8.805	56.817	1.00	11.60	ACPS
ATOM	821	CD2	HIS	105	-7.921	9.254	55.663	1.00	13.08	ACPS
ATOM	822	ND1	HIS	105	-6.442	9.749	57.192	1.00	11.93	ACPS
ATOM	823	CE1	HIS	105	-6.427	10.729	56.305	1.00	11.86	ACPS
ATOM	824	NE2	HIS	105	-7.315	10.451	55.366	1.00	12.18	ACPS
ATOM	825	C	HIS	105	-6.986	5.299	58.314	1.00	11.03	ACPS
ATOM	826	O	HIS	105	-7.888	4.471	58.165	1.00	12.54	ACPS
ATOM	827	N	THR	106	-6.165	5.309	59.367	1.00	11.51	ACPS
ATOM	828	CA	THR	106	-6.349	4.411	60.509	1.00	11.59	ACPS
ATOM	829	CB	THR	106	-5.289	3.270	60.620	1.00	11.24	ACPS
ATOM	830	OG1	THR	106	-4.065	3.780	61.169	1.00	11.20	ACPS
ATOM	831	CG2	THR	106	-5.017	2.634	59.261	1.00	12.65	ACPS
ATOM	832	C	THR	106	-6.225	5.273	61.771	1.00	12.23	ACPS
ATOM	833	O	THR	106	-6.002	6.482	61.692	1.00	12.54	ACPS
ATOM	834	N	LYS	107	-6.364	4.634	62.929	1.00	12.39	ACPS
ATOM	835	CA	LYS	107	-6.269	5.295	64.229	1.00	12.12	ACPS
ATOM	836	CB	LYS	107	-6.473	4.242	65.326	1.00	12.29	ACPS
ATOM	837	CG	LYS	107	-5.379	3.146	65.280	1.00	13.31	ACPS
ATOM	838	CD	LYS	107	-5.653	1.939	66.203	1.00	14.42	ACPS
ATOM	839	CE	LYS	107	-4.660	0.799	65.876	1.00	15.82	ACPS
ATOM	840	NZ	LYS	107	-4.895	-0.473	66.648	1.00	18.55	ACPS
ATOM	841	C	LYS	107	-4.936	5.998	64.490	1.00	12.43	ACPS
ATOM	842	O	LYS	107	-4.874	6.970	65.263	1.00	14.30	ACPS
ATOM	843	N	GLU	108	-3.871	5.516	63.857	1.00	11.38	ACPS
ATOM	844	CA	GLU	108	-2.540	6.061	64.099	1.00	11.08	ACPS
ATOM	845	CB	GLU	108	-1.692	4.997	64.823	1.00	10.76	ACPS
ATOM	846	CG	GLU	108	-1.320	3.790	63.936	1.00	11.72	ACPS
ATOM	847	CD	GLU	108	-0.835	2.550	64.706	1.00	11.82	ACPS
ATOM	848	OE1	GLU	108	-0.047	2.673	65.664	1.00	12.16	ACPS
ATOM	849	OE2	GLU	108	-1.224	1.420	64.329	1.00	11.39	ACPS
ATOM	850	C	GLU	108	-1.788	6.517	62.858	1.00	10.37	ACPS
ATOM	851	O	GLU	108	-0.769	7.193	62.977	1.00	10.85	ACPS
ATOM	852	N	TYR	109	-2.292	6.164	61.676	1.00	10.03	ACPS
ATOM	853	CA	TYR	109	-1.608	6.482	60.421	1.00	9.03	ACPS
ATOM	854	CB	TYR	109	-1.061	5.195	59.757	1.00	10.14	ACPS
ATOM	855	CG	TYR	109	-0.074	4.364	60.537	1.00	9.25	ACPS
ATOM	856	CD1	TYR	109	1.091	4.927	61.043	1.00	9.05	ACPS
ATOM	857	CE1	TYR	109	2.032	4.157	61.725	1.00	10.07	ACPS
ATOM	858	CD2	TYR	109	-0.283	2.996	60.730	1.00	10.49	ACPS
ATOM	859	CE2	TYR	109	0.649	2.217	61.410	1.00	10.01	ACPS
ATOM	860	CZ	TYR	109	1.807	2.809	61.902	1.00	11.02	ACPS
ATOM	861	OH	TYR	109	2.753	2.042	62.546	1.00	11.45	ACPS
ATOM	862	C	TYR	109	-2.487	7.101	59.343	1.00	9.01	ACPS
ATOM	863	O	TYR	109	-3.708	6.991	59.375	1.00	9.80	ACPS
ATOM	864	N	ALA	110	-1.825	7.735	58.381	1.00	9.15	ACPS

FIG. 2A-16

ATOM	865	CA	ALA	110	-2.475	8.207	57.162	1.00 10.18	ACPS
ATOM	866	CB	ALA	110	-2.489	9.726	57.072	1.00 9.95	ACPS
ATOM	867	C	ALA	110	-1.529	7.598	56.110	1.00 8.99	ACPS
ATOM	868	O	ALA	110	-0.322	7.843	56.143	1.00 10.23	ACPS
ATOM	869	N	ALA	111	-2.067	6.776	55.209	1.00 9.06	ACPS
ATOM	870	CA	ALA	111	-1.255	6.109	54.181	1.00 9.24	ACPS
ATOM	871	CB	ALA	111	-1.319	4.577	54.371	1.00 9.27	ACPS
ATOM	872	C	ALA	111	-1.710	6.462	52.773	1.00 9.10	ACPS
ATOM	873	O	ALA	111	-2.877	6.780	52.551	1.00 9.14	ACPS
ATOM	874	N	ALA	112	-0.782	6.399	51.822	1.00 9.52	ACPS
ATOM	875	CA	ALA	112	-1.107	6.713	50.434	1.00 9.40	ACPS
ATOM	876	CB	ALA	112	-0.973	8.219	50.190	1.00 10.40	ACPS
ATOM	877	C	ALA	112	-0.202	5.984	49.462	1.00 9.11	ACPS
ATOM	878	O	ALA	112	0.890	5.548	49.814	1.00 9.27	ACPS
ATOM	879	N	GLN	113	-0.680	5.843	48.233	1.00 10.03	ACPS
ATOM	880	CA	GLN	113	0.124	5.246	47.171	1.00 10.71	ACPS
ATOM	881	CB	GLN	113	-0.221	3.768	46.949	1.00 12.50	ACPS
ATOM	882	CG	GLN	113	-1.607	3.525	46.382	1.00 14.15	ACPS
ATOM	883	CD	GLN	113	-1.910	2.053	46.181	1.00 16.57	ACPS
ATOM	884	OE1	GLN	113	-2.978	1.699	45.686	1.00 17.95	ACPS
ATOM	885	NE2	GLN	113	-0.978	1.187	46.581	1.00 19.32	ACPS
ATOM	886	C	GLN	113	-0.088	6.047	45.884	1.00 10.42	ACPS
ATOM	887	O	GLN	113	-1.121	6.698	45.701	1.00 11.38	ACPS
ATOM	888	N	VAL	114	0.905	5.998	45.002	1.00 10.88	ACPS
ATOM	889	CA	VAL	114	0.872	6.727	43.742	1.00 11.50	ACPS
ATOM	890	CB	VAL	114	1.770	8.002	43.834	1.00 12.48	ACPS
ATOM	891	CG1	VAL	114	1.994	8.613	42.444	1.00 12.51	ACPS
ATOM	892	CG2	VAL	114	1.144	9.013	44.779	1.00 11.66	ACPS
ATOM	893	C	VAL	114	1.409	5.888	42.589	1.00 11.78	ACPS
ATOM	894	O	VAL	114	2.295	5.055	42.772	1.00 11.30	ACPS
ATOM	895	N	VAL	115	0.839	6.099	41.405	1.00 12.16	ACPS
ATOM	896	CA	VAL	115	1.322	5.454	40.195	1.00 12.60	ACPS
ATOM	897	CB	VAL	115	0.426	4.301	39.706	1.00 12.42	ACPS
ATOM	898	CG1	VAL	115	0.957	3.778	38.377	1.00 14.70	ACPS
ATOM	899	CG2	VAL	115	0.388	3.172	40.736	1.00 12.57	ACPS
ATOM	900	C	VAL	115	1.364	6.525	39.109	1.00 12.96	ACPS
ATOM	901	O	VAL	115	0.351	7.167	38.821	1.00 13.15	ACPS
ATOM	902	N	ILE	116	2.547	6.732	38.534	1.00 13.59	ACPS
ATOM	903	CA	ILE	116	2.736	7.708	37.454	1.00 15.01	ACPS
ATOM	904	CB	ILE	116	4.044	8.514	37.619	1.00 15.13	ACPS
ATOM	905	CG2	ILE	116	4.252	9.422	36.391	1.00 15.76	ACPS
ATOM	906	CG1	ILE	116	4.011	9.353	38.901	1.00 14.74	ACPS
ATOM	907	CD1	ILE	116	5.326	10.082	39.168	1.00 15.57	ACPS
ATOM	908	C	ILE	116	2.881	6.907	36.164	1.00 16.45	ACPS
ATOM	909	O	ILE	116	3.750	6.032	36.076	1.00 16.35	ACPS
ATOM	910	N	GLU	117	2.054	7.205	35.165	1.00 18.81	ACPS
ATOM	911	CA	GLU	117	2.142	6.481	33.894	1.00 21.39	ACPS
ATOM	912	CB	GLU	117	0.760	6.363	33.245	1.00 22.18	ACPS
ATOM	913	CG	GLU	117	-0.272	5.679	34.124	1.00 23.46	ACPS
ATOM	914	CD	GLU	117	-1.560	5.358	33.391	1.00 24.48	ACPS
ATOM	915	OE1	GLU	117	-1.582	4.373	32.622	1.00 25.10	ACPS
ATOM	916	OE2	GLU	117	-2.550	6.092	33.580	1.00 25.49	ACPS
ATOM	917	C	GLU	117	3.097	7.186	32.938	1.00 23.33	ACPS
ATOM	918	O	GLU	117	3.386	8.367	33.101	1.00 23.55	ACPS
ATOM	919	N	ALA	118	3.596	6.460	31.943	1.00 25.38	ACPS
ATOM	920	CA	ALA	118	4.516	7.055	30.979	1.00 27.43	ACPS
ATOM	921	CB	ALA	118	4.977	6.002	29.985	1.00 27.34	ACPS

FIG. 2A-17

ATOM	922	C	ALA	118	3.841	8.208	30.244	1.00 28.57	ACPS
ATOM	923	OT1	ALA	118	2.598	8.169	30.110	1.00 29.57	ACPS
ATOM	924	OT2	ALA	118	4.563	9.133	29.800	1.00 30.29	ACPS
ATOM	925	O	HOH	1	8.184	16.571	66.146	1.00 24.49	WAT
ATOM	926	O	HOH	2	8.785	8.855	56.929	1.00 23.58	WAT
ATOM	927	O	HOH	3	-6.634	6.371	40.520	1.00 13.40	WAT
ATOM	928	O	HOH	4	6.850	6.588	56.334	1.00 12.56	WAT
ATOM	929	O	HOH	5	-8.045	6.689	43.987	1.00 13.42	WAT
ATOM	930	O	HOH	6	-5.322	9.243	59.567	1.00 14.25	WAT
ATOM	931	O	HOH	7	-8.408	6.897	46.767	1.00 10.54	WAT
ATOM	932	O	HOH	8	0.163	8.272	65.337	1.00 14.13	WAT
ATOM	933	O	HOH	9	-14.561	9.350	40.005	1.00 16.00	WAT
ATOM	934	O	HOH	10	5.984	9.787	56.562	1.00 12.10	WAT
ATOM	935	O	HOH	11	9.603	20.654	50.362	1.00 18.90	WAT
ATOM	936	O	HOH	12	9.199	12.001	56.416	1.00 20.43	WAT
ATOM	937	O	HOH	13	-5.501	13.397	53.431	1.00 13.06	WAT
ATOM	938	O	HOH	14	-2.767	25.961	44.622	1.00 17.37	WAT
ATOM	939	O	HOH	15	1.460	20.979	40.473	1.00 16.78	WAT
ATOM	940	O	HOH	16	-6.412	20.992	45.756	1.00 19.74	WAT
ATOM	941	O	HOH	17	-6.145	9.042	41.305	1.00 12.90	WAT
ATOM	942	O	HOH	18	-0.223	24.078	42.670	1.00 18.93	WAT
ATOM	943	O	HOH	19	-7.596	19.455	37.156	1.00 19.34	WAT
ATOM	944	O	HOH	20	-5.063	33.496	51.266	1.00 22.07	WAT
ATOM	945	O	HOH	21	-1.492	0.933	67.571	1.00 14.90	WAT
ATOM	946	O	HOH	22	10.843	7.091	38.836	1.00 23.19	WAT
ATOM	947	O	HOH	23	1.577	14.422	68.706	1.00 24.82	WAT
ATOM	948	O	HOH	24	-7.606	8.898	61.270	1.00 18.79	WAT
ATOM	949	O	HOH	25	0.081	9.327	35.513	1.00 22.45	WAT
ATOM	950	O	HOH	26	-6.295	18.339	48.365	1.00 15.49	WAT
ATOM	951	O	HOH	27	-0.673	19.887	66.759	1.00 21.01	WAT
ATOM	952	O	HOH	28	2.234	22.708	42.588	1.00 18.21	WAT
ATOM	953	O	HOH	29	5.866	5.790	62.516	1.00 18.49	WAT
ATOM	954	O	HOH	30	0.991	15.961	36.660	1.00 18.35	WAT
ATOM	955	O	HOH	31	-6.406	9.357	38.563	1.00 20.48	WAT
ATOM	956	O	HOH	32	-11.957	11.623	37.352	1.00 24.33	WAT
ATOM	957	O	HOH	33	-10.389	14.434	49.725	1.00 27.42	WAT
ATOM	958	O	HOH	34	-4.448	20.165	63.854	1.00 24.32	WAT
ATOM	959	O	HOH	35	1.450	2.725	43.903	1.00 20.38	WAT
ATOM	960	O	HOH	36	-9.847	19.977	43.739	1.00 23.75	WAT
ATOM	961	O	HOH	37	-4.274	35.006	45.404	1.00 20.66	WAT
ATOM	962	O	HOH	38	-0.833	22.659	40.326	1.00 19.80	WAT
ATOM	963	O	HOH	39	-10.345	18.568	67.239	1.00 20.80	WAT
ATOM	964	O	HOH	40	-8.477	13.551	55.975	1.00 26.24	WAT
ATOM	965	O	HOH	41	-5.655	29.371	49.873	1.00 28.51	WAT
ATOM	966	O	HOH	42	-10.675	16.934	50.659	1.00 24.92	WAT
ATOM	967	O	HOH	43	-12.936	12.520	51.596	1.00 27.30	WAT
ATOM	968	O	HOH	44	5.317	21.159	39.730	1.00 21.12	WAT
ATOM	969	O	HOH	45	-16.788	9.865	48.461	1.00 26.54	WAT
ATOM	970	O	HOH	46	-11.077	6.886	57.927	1.00 23.02	WAT
ATOM	971	O	HOH	47	8.239	21.236	62.377	1.00 34.53	WAT
ATOM	972	O	HOH	48	-12.230	29.900	51.577	1.00 21.86	WAT
ATOM	973	O	HOH	49	14.440	16.080	45.556	1.00 23.96	WAT
ATOM	974	O	HOH	50	12.861	21.772	39.431	1.00 30.68	WAT
ATOM	975	O	HOH	51	-14.091	19.163	60.526	1.00 27.55	WAT
ATOM	976	O	HOH	52	6.663	27.800	61.179	1.00 32.84	WAT
ATOM	977	O	HOH	53	-11.635	27.871	53.345	1.00 31.03	WAT
ATOM	978	O	HOH	54	-6.997	7.591	67.044	1.00 25.57	WAT

FIG. 2A-18

ATOM	979	O	HOH	55	5.799	6.629	59.843	1.00	16.31	WAT
ATOM	980	O	HOH	56	2.012	25.703	66.142	1.00	35.32	WAT
ATOM	981	O	HOH	57	0.121	2.727	31.610	1.00	42.03	WAT
ATOM	982	O	HOH	58	1.534	10.328	32.415	1.00	41.42	WAT
ATOM	983	O	HOH	59	-16.524	4.165	56.298	1.00	21.92	WAT
ATOM	984	O	HOH	60	-13.305	16.632	64.615	1.00	23.56	WAT
ATOM	985	O	HOH	61	-12.177	16.550	67.442	1.00	20.64	WAT
ATOM	986	O	HOH	62	-14.009	9.985	52.284	1.00	25.38	WAT
ATOM	987	O	HOH	63	-9.900	9.225	59.680	1.00	23.49	WAT
ATOM	988	O	HOH	64	-6.771	33.311	45.569	1.00	21.83	WAT
ATOM	989	O	HOH	65	-2.713	20.087	61.546	1.00	24.39	WAT
ATOM	990	O	HOH	66	-7.980	17.897	68.615	1.00	22.87	WAT
ATOM	991	O	HOH	67	-13.405	7.809	38.191	1.00	26.90	WAT
ATOM	992	O	HOH	68	-4.952	28.402	44.638	1.00	33.63	WAT
ATOM	993	O	HOH	69	-2.685	3.686	68.288	1.00	31.25	WAT
ATOM	994	O	HOH	70	8.512	9.048	60.830	1.00	28.65	WAT
ATOM	995	O	HOH	71	-1.486	18.163	62.740	1.00	32.45	WAT
ATOM	996	O	HOH	72	5.603	18.678	70.084	1.00	26.38	WAT
ATOM	997	O	HOH	73	-7.547	29.689	51.621	1.00	29.41	WAT
ATOM	998	O	HOH	74	10.855	19.331	52.981	1.00	26.05	WAT
ATOM	999	O	HOH	75	-11.689	10.901	61.337	1.00	28.27	WAT
ATOM	1000	O	HOH	76	-0.166	23.981	38.303	1.00	33.92	WAT
ATOM	1001	O	HOH	77	-11.224	22.643	66.111	1.00	30.50	WAT
ATOM	1002	O	HOH	78	15.942	18.609	39.466	1.00	35.09	WAT
ATOM	1003	O	HOH	79	-9.721	15.254	57.360	1.00	23.81	WAT
ATOM	1004	O	HOH	80	-9.623	11.467	57.685	1.00	26.57	WAT
ATOM	1005	O	HOH	81	-10.600	4.395	59.079	1.00	26.62	WAT
ATOM	1006	O	HOH	82	-8.498	10.896	38.078	1.00	35.64	WAT
ATOM	1007	O	HOH	83	-2.753	18.652	65.536	1.00	26.51	WAT
ATOM	1008	O	HOH	84	9.568	24.455	43.921	1.00	31.56	WAT
ATOM	1009	O	HOH	85	19.835	12.684	45.040	1.00	35.96	WAT
ATOM	1010	O	HOH	86	13.338	21.812	46.003	1.00	39.76	WAT
ATOM	1011	O	HOH	87	11.096	20.032	59.974	1.00	34.99	WAT
ATOM	1012	O	HOH	88	3.720	23.855	40.646	1.00	31.59	WAT
ATOM	1013	O	HOH	89	-1.224	22.461	66.261	1.00	34.76	WAT
ATOM	1014	O	HOH	90	-7.691	9.770	63.766	1.00	31.45	WAT
ATOM	1015	O	HOH	91	17.406	11.773	44.998	1.00	29.99	WAT
ATOM	1016	O	HOH	92	-1.506	7.951	67.587	1.00	28.61	WAT
ATOM	1017	O	HOH	93	-3.462	10.383	67.429	1.00	32.97	WAT
ATOM	1018	O	HOH	94	-2.310	12.680	66.265	1.00	27.88	WAT
ATOM	1019	O	HOH	95	-4.299	16.505	66.744	1.00	34.32	WAT
ATOM	1020	O	HOH	96	0.990	24.911	62.972	1.00	31.02	WAT
ATOM	1021	O	HOH	97	-13.635	13.854	63.282	1.00	15.69	WAT
ATOM	1022	O	HOH	98	-12.472	13.178	48.835	1.00	25.84	WAT
ATOM	1023	O	HOH	99	0.796	0.192	42.865	1.00	28.22	WAT
ATOM	1024	N1	COA	120	-12.948	7.608	44.920	1.00	13.13	COA
ATOM	1025	C2	COA	120	-11.643	7.336	45.414	1.00	12.29	COA
ATOM	1026	N3	COA	120	-11.182	7.731	46.667	1.00	13.13	COA
ATOM	1027	C4	COA	120	-12.090	8.415	47.420	1.00	12.87	COA
ATOM	1028	C5	COA	120	-13.461	8.771	47.064	1.00	12.68	COA
ATOM	1029	C6	COA	120	-13.899	8.321	45.698	1.00	13.32	COA
ATOM	1030	N6	COA	120	-15.094	8.573	45.246	1.00	13.97	COA
ATOM	1031	N7	COA	120	-14.087	9.450	48.042	1.00	13.45	COA
ATOM	1032	C8	COA	120	-13.179	9.555	49.021	1.00	14.05	COA
ATOM	1033	N9	COA	120	-11.940	8.949	48.707	1.00	12.82	COA
ATOM	1034	C1*	COA	120	-10.508	8.739	49.433	1.00	12.92	COA
ATOM	1035	C2*	COA	120	-10.131	10.063	49.988	1.00	12.61	COA

FIG. 2A-19


```
ATOM   1036  O2*  COA   120      -8.885  10.585  49.617  1.00 13.09      COA
ATOM   1037  C3*  COA   120     -10.321   9.967  51.470  1.00 12.95      COA
ATOM   1038  O3*  COA   120      -9.269  10.478  52.488  1.00 12.93      COA
ATOM   1039  P3*  COA   120      -9.182  12.127  52.589  1.00 13.47      COA
ATOM   1040  O7   COA   120      -8.835  12.768  51.184  1.00 13.51      COA
ATOM   1041  O8   COA   120      -8.049  12.448  53.626  1.00 13.28      COA
ATOM   1042  O9   COA   120     -10.609  12.596  53.131  1.00 14.44      COA
ATOM   1043  C4*  COA   120     -10.208   8.375  51.725  1.00 13.08      COA
ATOM   1044  O4*  COA   120     -10.977   7.897  50.509  1.00 12.26      COA
ATOM   1045  C5*  COA   120     -10.401   7.949  53.127  1.00 14.58      COA
ATOM   1046  O5*  COA   120     -10.469   6.473  52.938  1.00 13.48      COA
ATOM   1047  P1   COA   120     -10.652   5.672  54.364  1.00 12.56      COA
ATOM   1048  O1   COA   120      -9.729   6.240  55.365  1.00 13.21      COA
ATOM   1049  O2   COA   120     -10.459   4.226  54.119  1.00 15.04      COA
ATOM   1050  O3   COA   120     -12.029   6.083  54.854  1.00 16.52      COA
ATOM   1051  P2   COA   120     -13.553   5.541  54.845  1.00 22.65      COA
ATOM   1052  O4   COA   120     -13.663   4.249  55.488  1.00 23.91      COA
ATOM   1053  O5   COA   120     -14.429   6.530  55.551  1.00 25.17      COA
ATOM   1054  O6   COA   120     -13.926   5.591  53.277  1.00 23.32      COA
ATOM   1055  C11  COA   120     -14.755   4.650  51.149  1.00 25.32      COA
ATOM   1056  C12  COA   120     -13.824   4.473  52.426  1.00 24.46      COA
ATOM   1057  C13  COA   120     -14.105   5.689  50.154  1.00 25.05      COA
ATOM   1058  C14  COA   120     -14.799   3.243  50.564  1.00 25.09      COA
ATOM   1059  C10  COA   120     -16.252   5.244  51.556  1.00 26.37      COA
ATOM   1060  O10  COA   120     -17.086   5.395  50.361  1.00 26.75      COA
ATOM   1061  C9   COA   120     -17.067   4.353  52.553  1.00 27.72      COA
ATOM   1062  O39  COA   120     -16.649   4.199  53.819  1.00 28.04      COA
ATOM   1063  N8   COA   120     -18.144   3.780  52.101  1.00 30.34      COA
ATOM   1064  C7   COA   120     -19.329   3.490  52.916  1.00 32.23      COA
ATOM   1065  C42  COA   120     -19.224   2.064  53.477  1.00 33.78      COA
ATOM   1066  C43  COA   120     -19.805   1.971  54.888  1.00 34.86      COA
ATOM   1067  O44  COA   120     -20.414   2.967  55.487  1.00 36.24      COA
ATOM   1068  N4   COA   120     -19.632   0.789  55.446  1.00 34.84      COA
ATOM   1069  C3   COA   120     -20.112   0.432  56.852  1.00 34.67      COA
ATOM   1070  C47  COA   120     -19.736  -0.998  57.112  1.00 34.47      COA
ATOM   1071  S1   COA   120     -20.877  -2.208  56.301  1.00 33.46      COA
ATOM   1072 CA+2 CA2     1       7.365   8.523  54.928  1.00 11.64      IONS
ATOM   1073 CL-1 CL1     2       5.841   9.868  59.601  1.00 16.02      IONS
ATOM   1074 CA+2 CA2     3       0.000   0.000  65.920  0.33  1.00      IONS
END
```

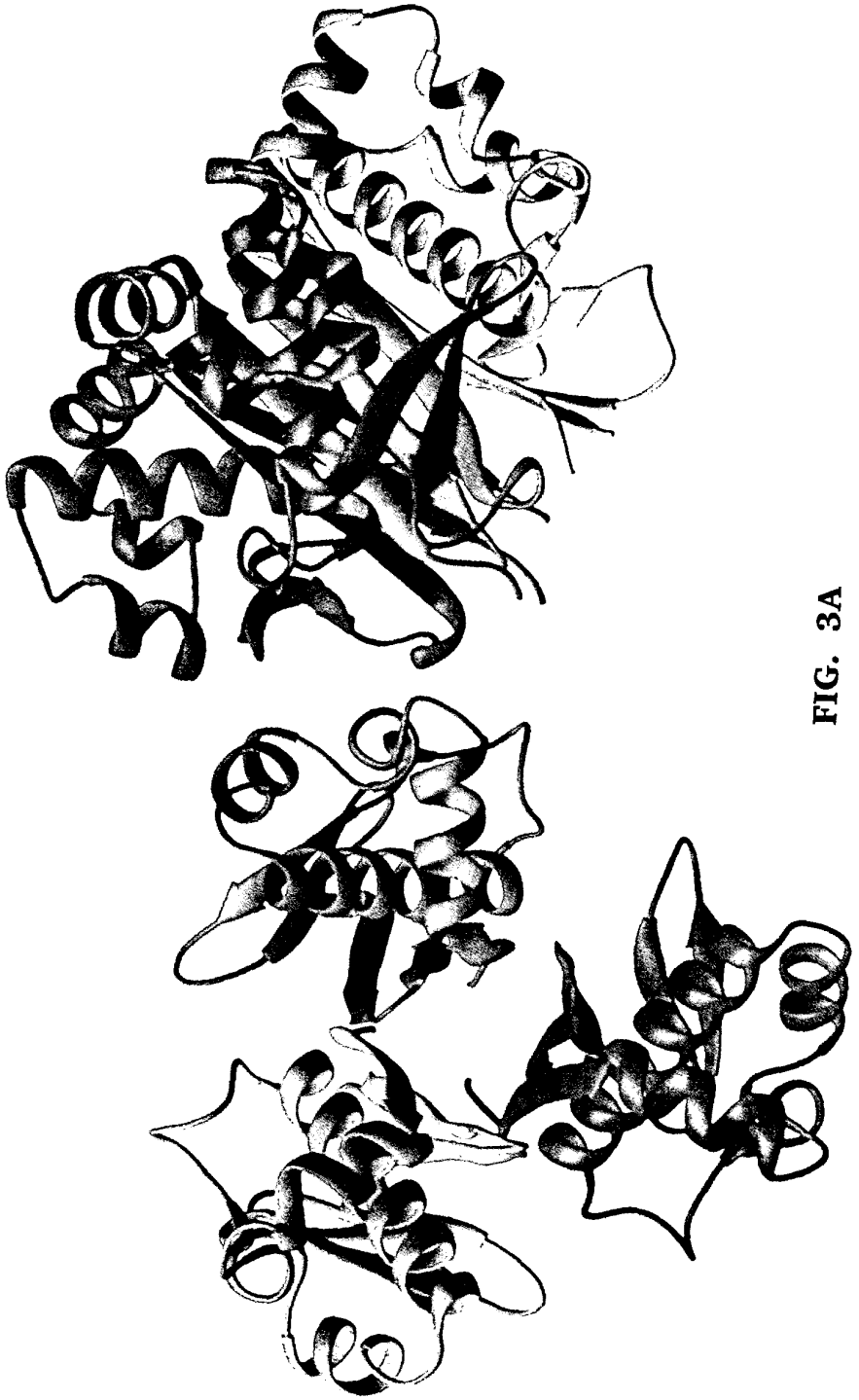
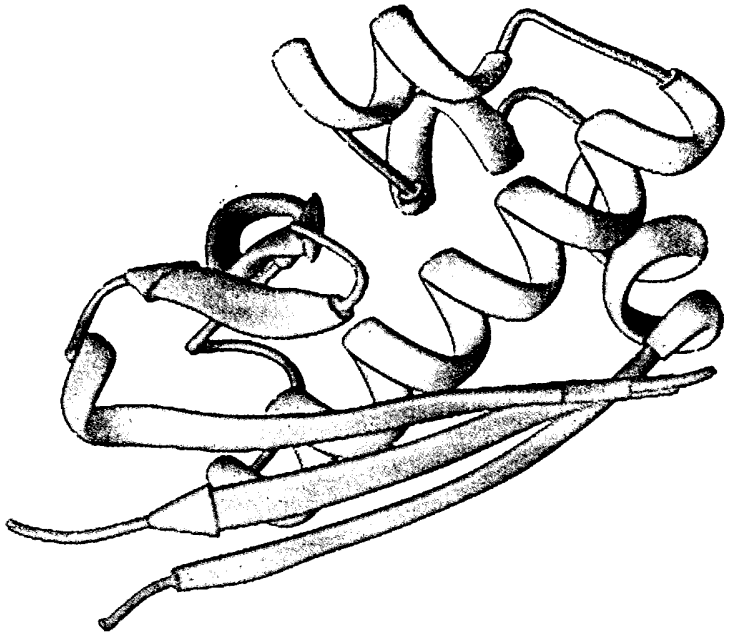


FIG. 3A



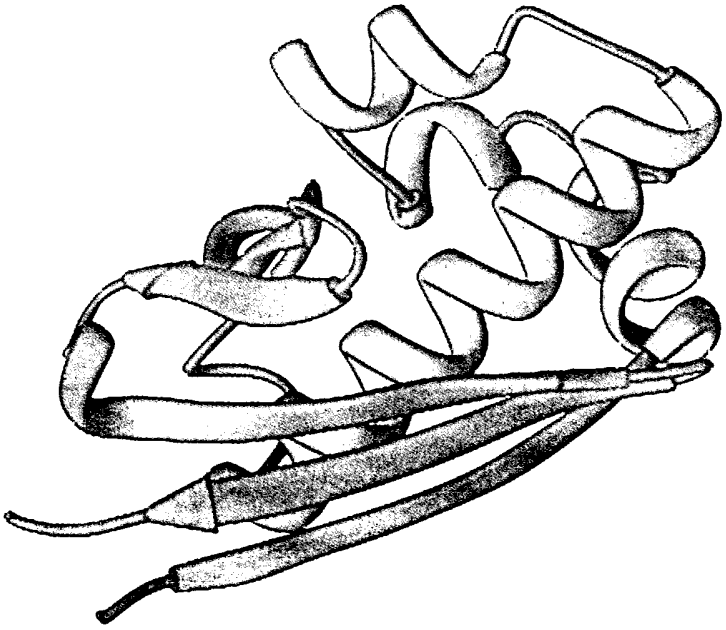


FIG. 3B

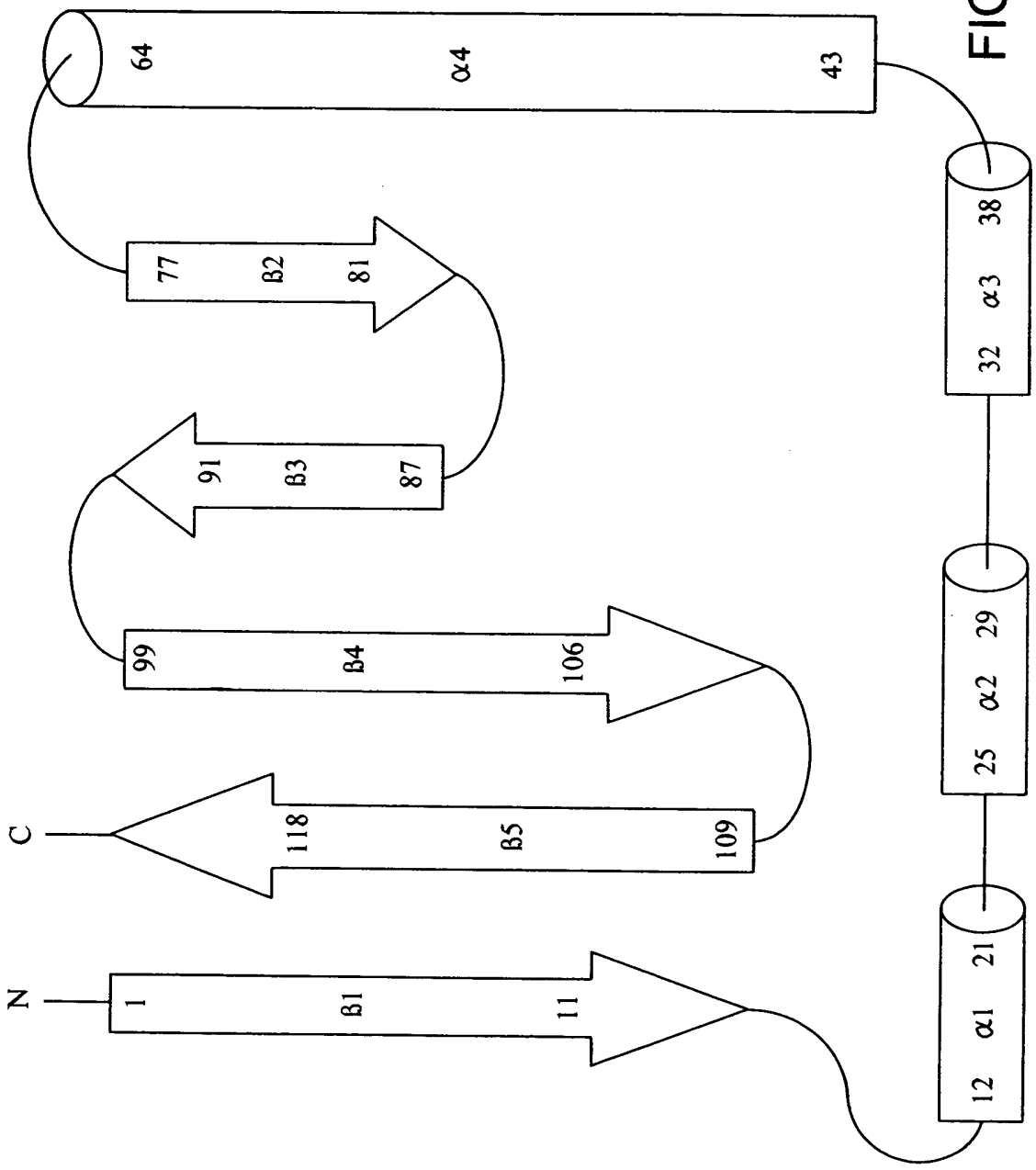


FIG. 3C

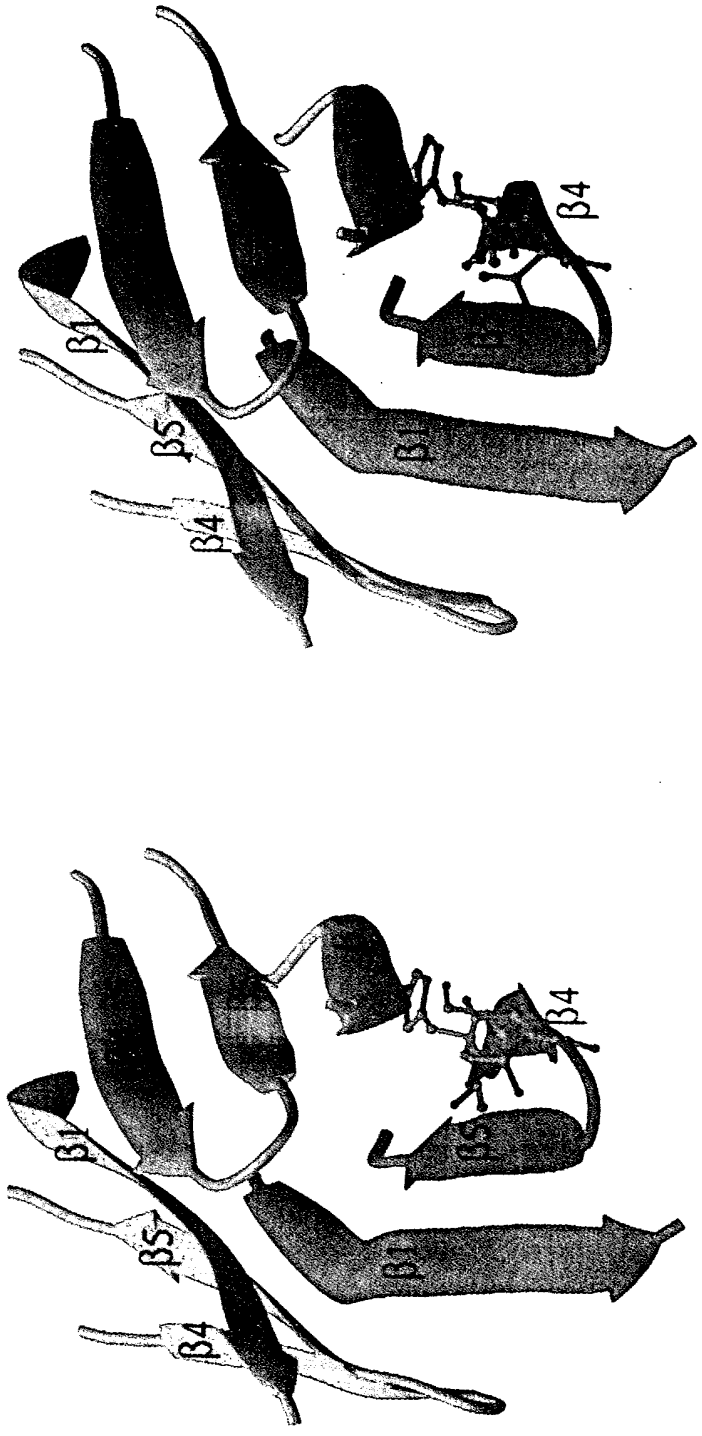


FIG. 4

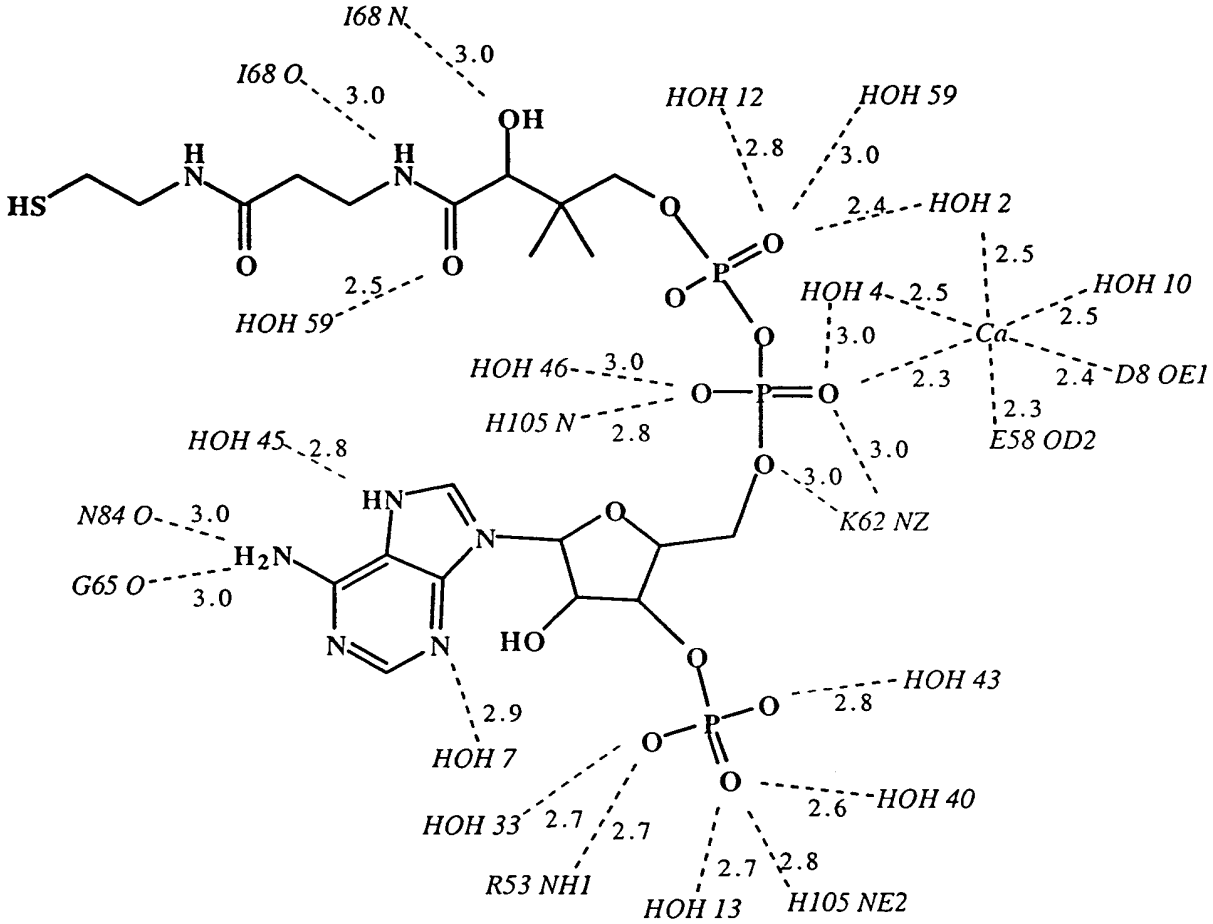


FIG. 5

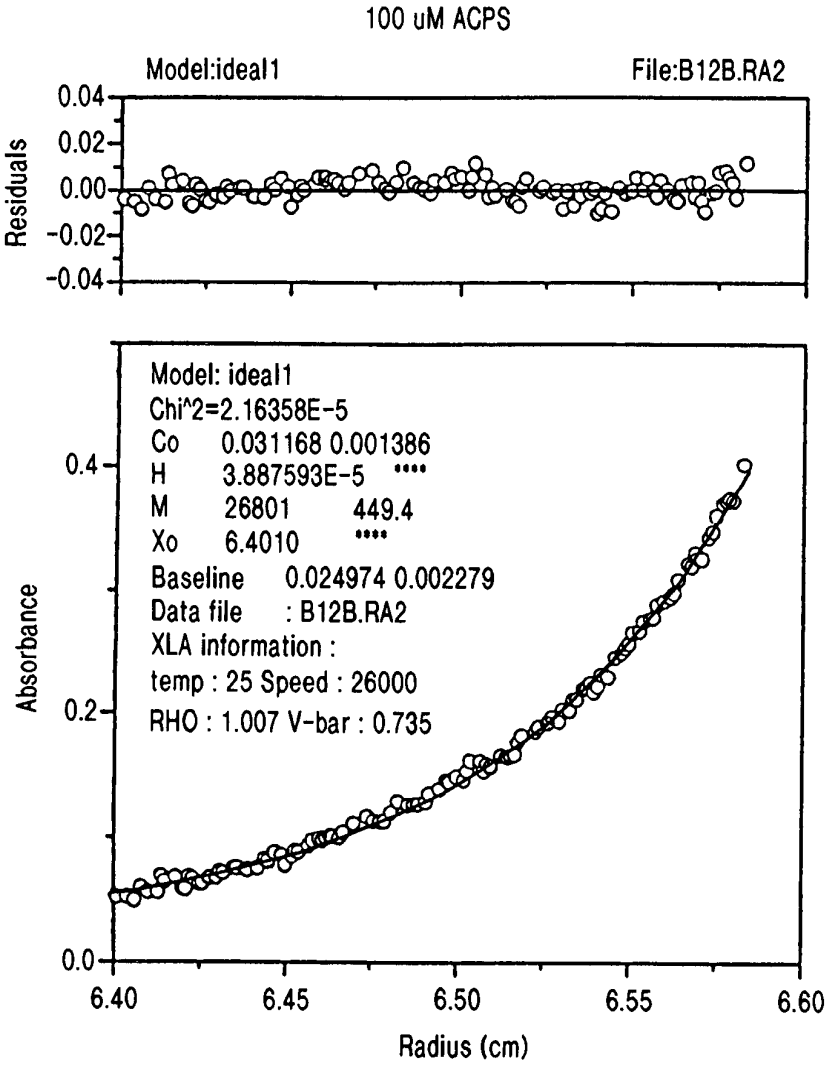


FIG. 6A

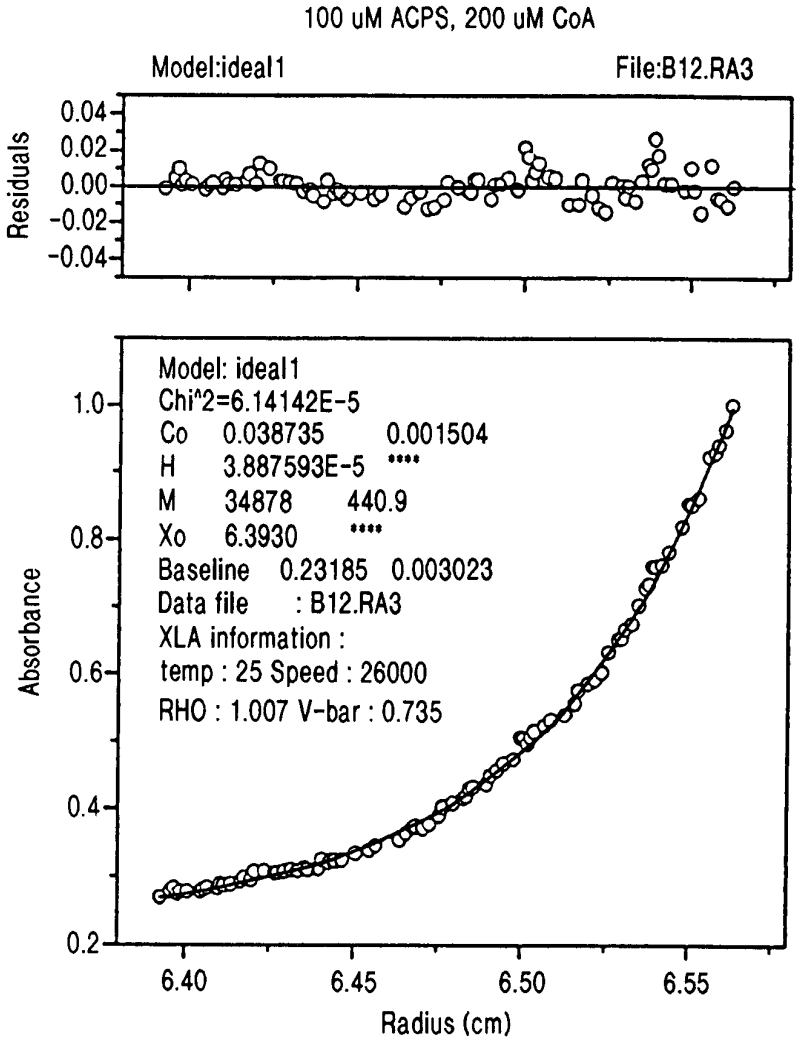
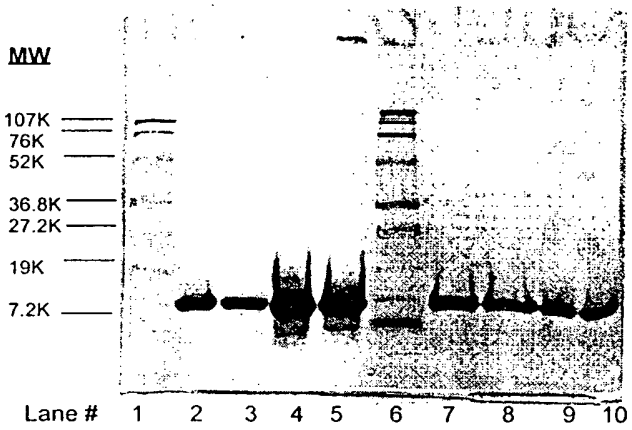


FIG. 6B

15% Non-reducing, denaturing gel of ACPS samples before and after analytical centrifugation



Lane #	ACPS samples
2	pH 5.2
3	pH 5.2, heated 10 min at 100 deg in gel sample buffer
4	pH 6.4, after sedimentation equilibrium expt.
5	pH 6.4, after equilibrium expt, heated 10 min at 100deg in gel buffer
7	pH 7.4
8	pH 7.4, heated 10 min at 100 deg in gel buffer
9	pH 6.4
10	pH 6.4, heated 10 min at 100 deg in gel sample buffer

Lanes 2, 3, 7, 8, 9, 10: 20 uL of a freshly prepared 32 ujM ACPS sample was added
Lanes 4, 5: 20 uL of the 100 uM ACPS pH 6.4 solution from the sedimentation equilbrium experiment was used

FIG. 7

MIYGI GLDIT ELKRI ASMAG RQKRF AERIL
TRSEL DQYYE LSEKR KNEFL AGRFA AKEAF
SKAFG TGIGR QLSFQ DIEIR KDQNG KPYII
CTKLS QAAVH VSITH TKEYA AAQVV IERLS
S

FIG. 8

```
Aquifex              1  ----MIGVDIVKNERIKDALERFGDKFLDRIYTKRELEYCY----AHCDFLPCLAARWAG
Chlamydophila        1  MEIIHIGTDIIEISRIREAIATHGNRLLNRIFTEAEQKYCL----EKTDPIPSFAGRFAG
Helicobacter         1  ----MIGIDIVSIARIEKCVKRFKMKFLERFLSPSEIVLCK----DKSS---SIAGFFAL
Staphylococcus       1  -MIHGIGVDLIEIDRIQALYSKQ-PKLVERILTKNEQHKFNN-FTHEQRKIEFLAGRFAT
Thermotoga           1  -MIVGVGIDVLEVERVP-------EKFAERILGESEKRLF---LTRKRRR-EFIAGRFAL
Escherichia          1  MAILGLGTDIVEIARIEAVIARSGDRLARRVLSDNEWAIWK---THHQPV-RFLAKRFAY
Rickettsia           1  -MLIGVGTDIVQIPRIEKILNIYQELFAKKILALKELKQFT--LLNKTNHATFLAKRFSA
Streptomyces         1  MSIIGVGIDVAEVERFGA-ALERTPALAGRLFLESELLLP----GGERRGVASLAARFAA
Treponema            1  -MIIGVGIDIVEIERFVS-WTHNVRLLR-RFFHQEEIVDF----FKNHMRAQFLATRFAA
Bacillus             1  -MIYGIGLDITELKRIAS-MAGRQKRFAERILTRSELDQYY--ELSEKRKNEFLAGRFAA
Bradyrhizobium       1  -MIIGIGSDLIDITRVGKVIERHGERFLDRIFTAAERAKAERRAKNEKMVVATYAKRFAA
Mycobacterium        1  MGIVGVGIDLVSIPDFAEQVSQPGTVFM-TIFTPGERRDAS---VKSSSAVCHLAARWAV
consensus            1        G D                              E                 A
                     1  1.....10.....20.....30.....40.....50.....

Aquifex             53  KEAVLKAFYTEFKIFL------RFKEIEILGNRGRPPTVVINRE--GVEEILKNY----E
Chlamydophila       57  KEAVAKALGTGIGSVV------AWKDIEVFKVSHGPEVLLPS----HVYAKIGIS----K
Helicobacter        50  KEACSKALQVGIGKEL------SFLDIKISKSPKNAPLITLSK---EKMDYFNIQ----S
Staphylococcus      58  KEAFSKALGTGLGKHV------AFNDIDCYNDELGKPKI----------DYEGF-----I
Thermotoga          49  KEAFFKALGTGLNGH-------SFTDVEFLESN-GKPVLCVH------KDFGFFN----Y
Escherichia         57  KEAAAKAFGTGIRNGL------AFNQFEVFNDELGKPRLRLWGEALKLAEKLGVA----N
Rickettsia          58  KEAVSKAFGVGIGRGI------NFKDITILNDNLGKPTVEISS---HYTNKLAPF----N
Streptomyces        56  KEALAKALGAPAG--L------LWTDAEVWVEAGGRPRLRVTGTVAARAAELGVA----S
Treponema           54  KEAFGKALGTGLRN-M------ELRNIRVCQNGWGKPRLEVYGAAQAMLAATGGT----H
Bacillus            57  KEAFSKAFGTGIGRQL------SFQDIEIRKDQNGKPYIICT--------KLSQA----A
Bradyrhizobium      60  KEACSKALGTGIRRGV------WWRDMGVVNLPGGRPTMQLTGGALARLQALTPDGFEAR
Mycobacterium       57  KEAVIKAWSGSRFAQRPMLPENIHRDIEVVNDMWGRPRVRLTG---AIAKHLTDV----T
consensus           61  KEA  KA
                    61  61.....70.....80.....90.....100.....110.....

Aquifex            101  VIVSLSHERDYSVAVAYIKKKS----------------------------------------
Chlamydophila      103  VILSISHCKEYATATAIALA------------------------------------------
Helicobacter        97  LSASISHDAGFAIAVVVVSSSNE---------------------------------------
Staphylococcus      97  VHVSISHTEHYAMSQVVLEK----------SAF-----------------------------
Thermotoga          91  AHVSLSH-DRFAVALVVLEKRKGDIIVEGDESFLRKRFEVLERSVEGWEIETSLPPFTLK
Escherichia        107  MHVTLADERHYACATVIIES-------------------------------------------
Rickettsia         105  IHLSLSDDYPICIAFAIIESNC----------------------------------------
Streptomyces       104  WHVSLSHDAGIASAVVIAEG-------------------------------------------
Treponema          103  IQVSLTHEREVASAIVIIEGEPL----------------------------------------
Cacillus            99  VHVSITHTKEYAAAQVVIERLSS----------------------------------------
Bradyrhizobium     114  IDVSITDDWPLAQAFVIISAVPLAKS-------------------------------------
Mycobacterium      110  IHVSLTHEGDIAAAVVILEVL------------------------------------------
consensus          121
                   121  121.....130.....140.....150.....160.....170.....

Aquifex                 ---------------------
Chlamydophila           ---------------------
Helicobacter            ---------------------
Staphylococcus          ---------------------
Thermotoga         150  KLLESSGCRLVRYGNILIGE
Excherichia             ---------------------
Rickettsia              ---------------------
Streptomyces            ---------------------
Treponema               ---------------------
Bacillus                ---------------------
Bradyrhizobium          ---------------------
Mycobacterium           ---------------------
consensus          181
                   181  181.....190.....
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FIG. 9